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Adjoint Sensitivity Analysis for Scale-Resolving Turbulent Flow Solvers

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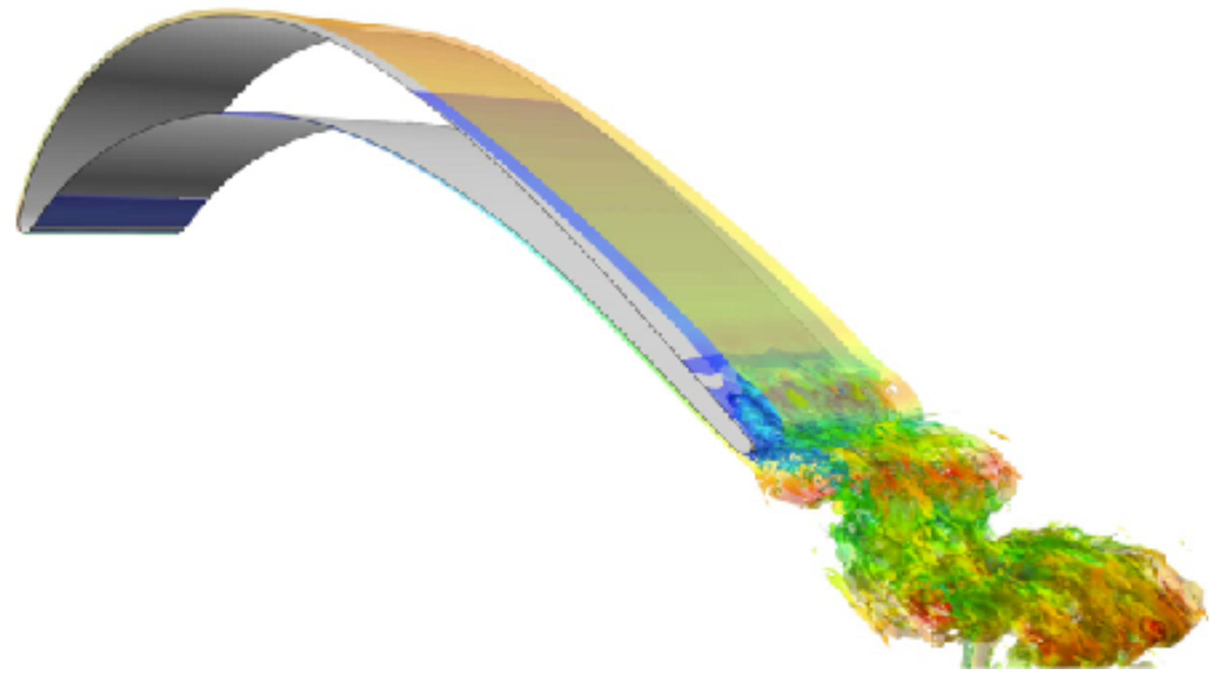
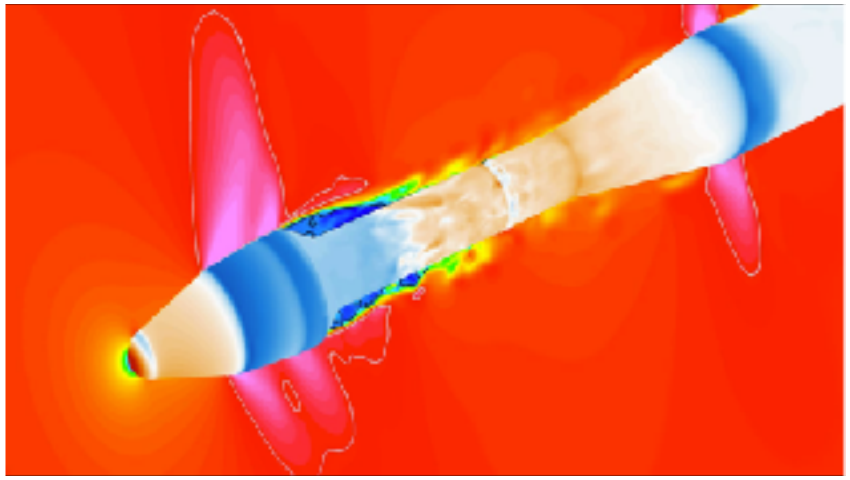
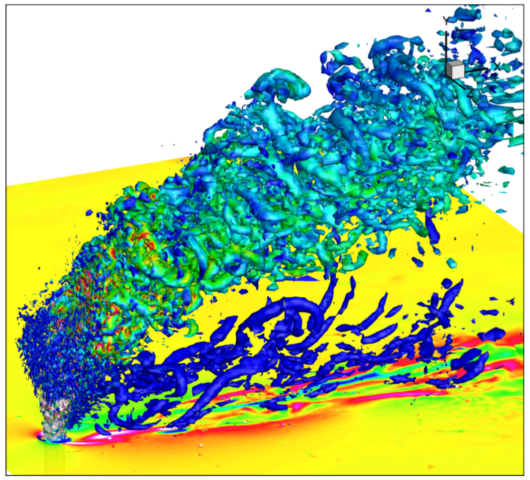
Adjoint Sensitivity Analysis of High Fidelity Simulations

- Types of Sensitivity Analysis
  - Tangent: sensitivity of many objectives to one input parameter
  - Adjoint: sensitivity of one objective to many input parameters
    - Gradient-based Design Optimization
    - Error Estimation
    - Mesh Adaptation
    - Uncertainty Quantification
- Systems with unsteady flows have many important objective functions that are time averaged

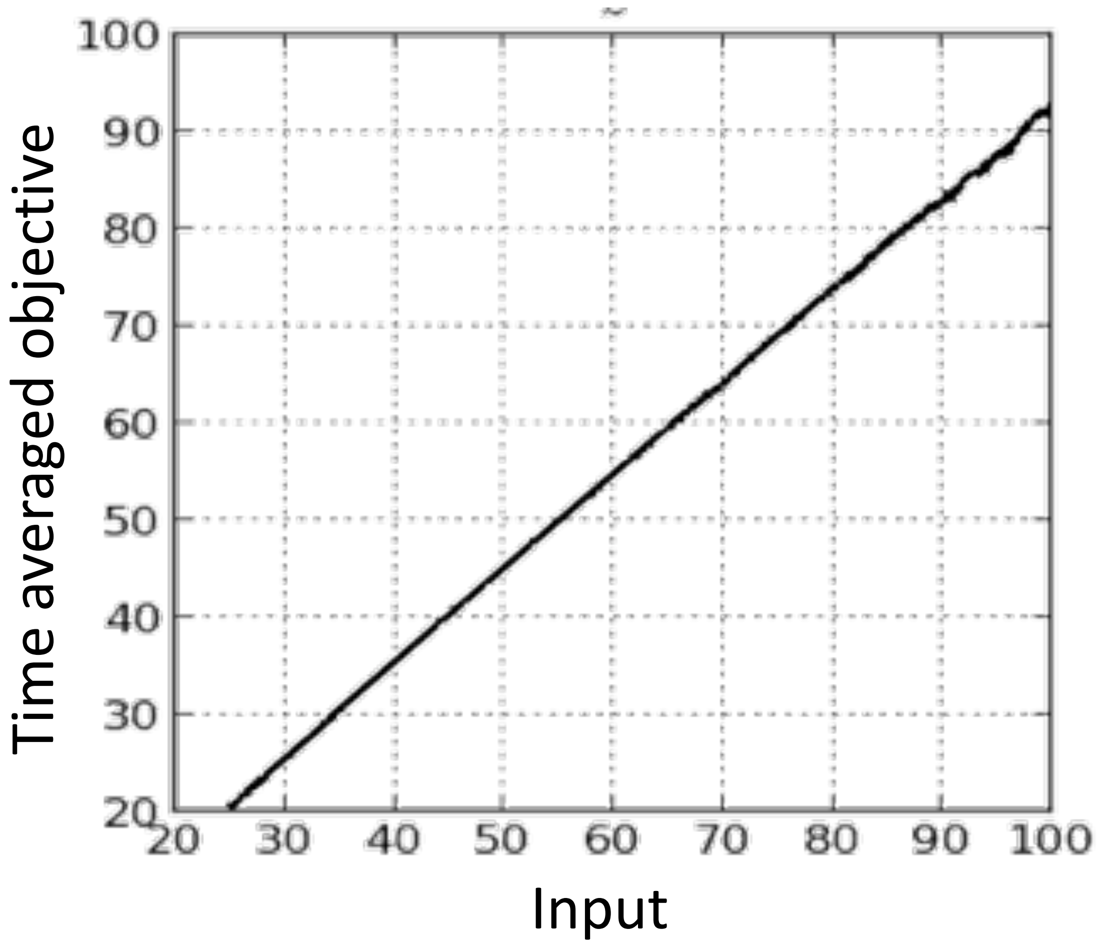


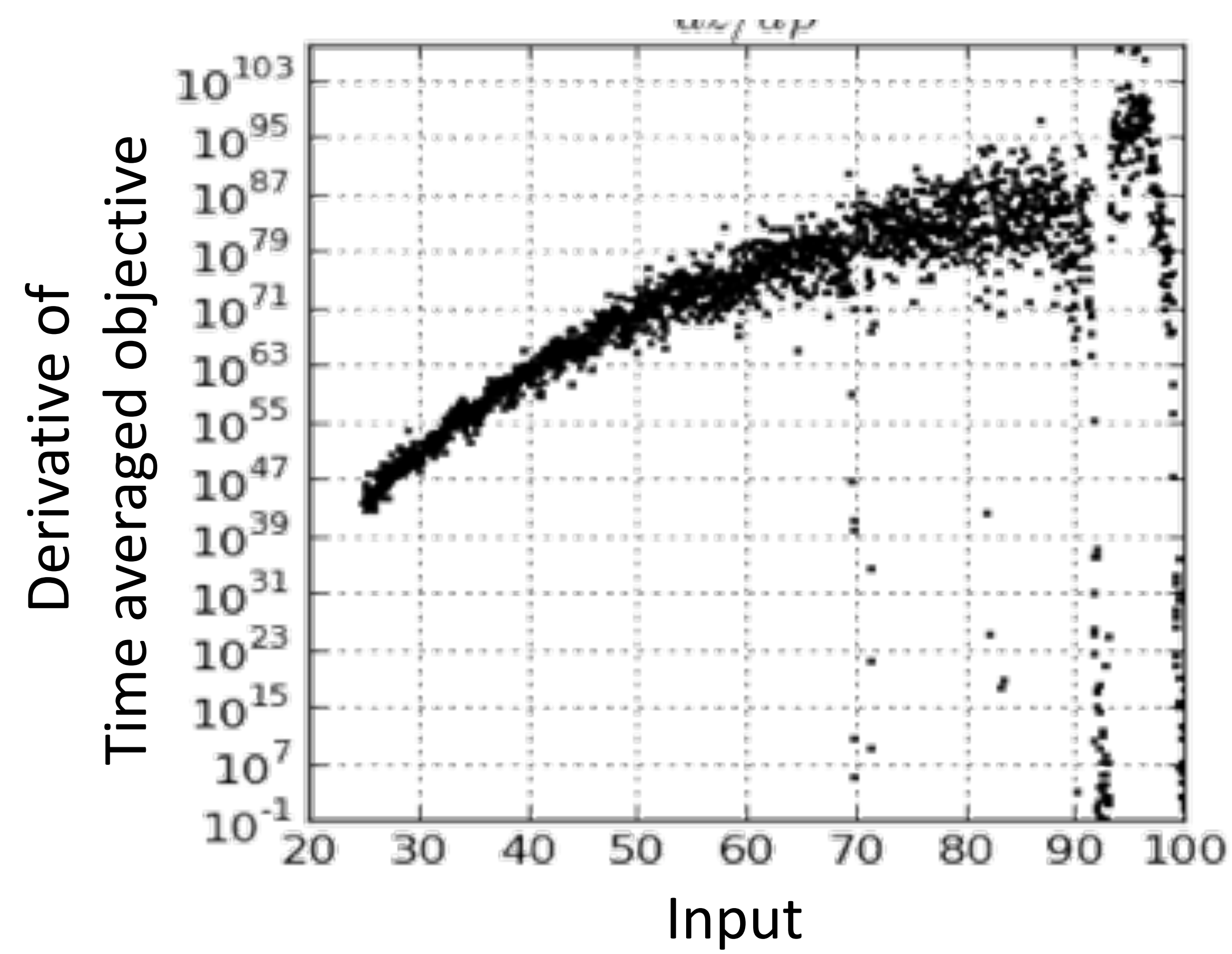


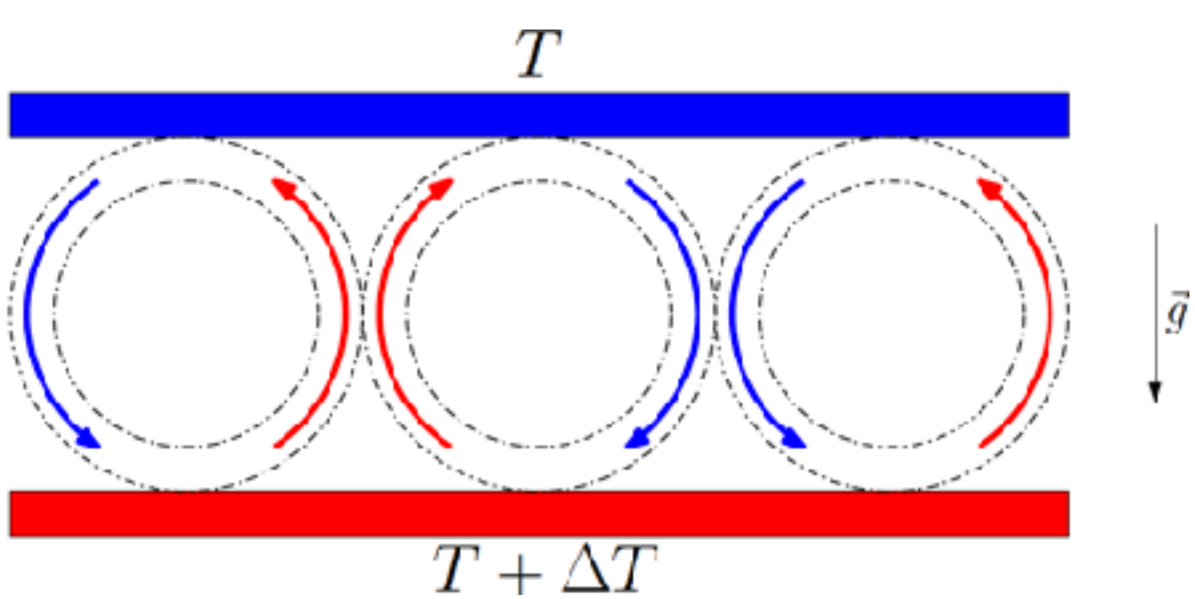


→ **Traditional sensitivity analysis fails for these objectives in high fidelity simulations, which exhibit chaotic dynamics**

Failure of conventional sensitivity analysis for chaos

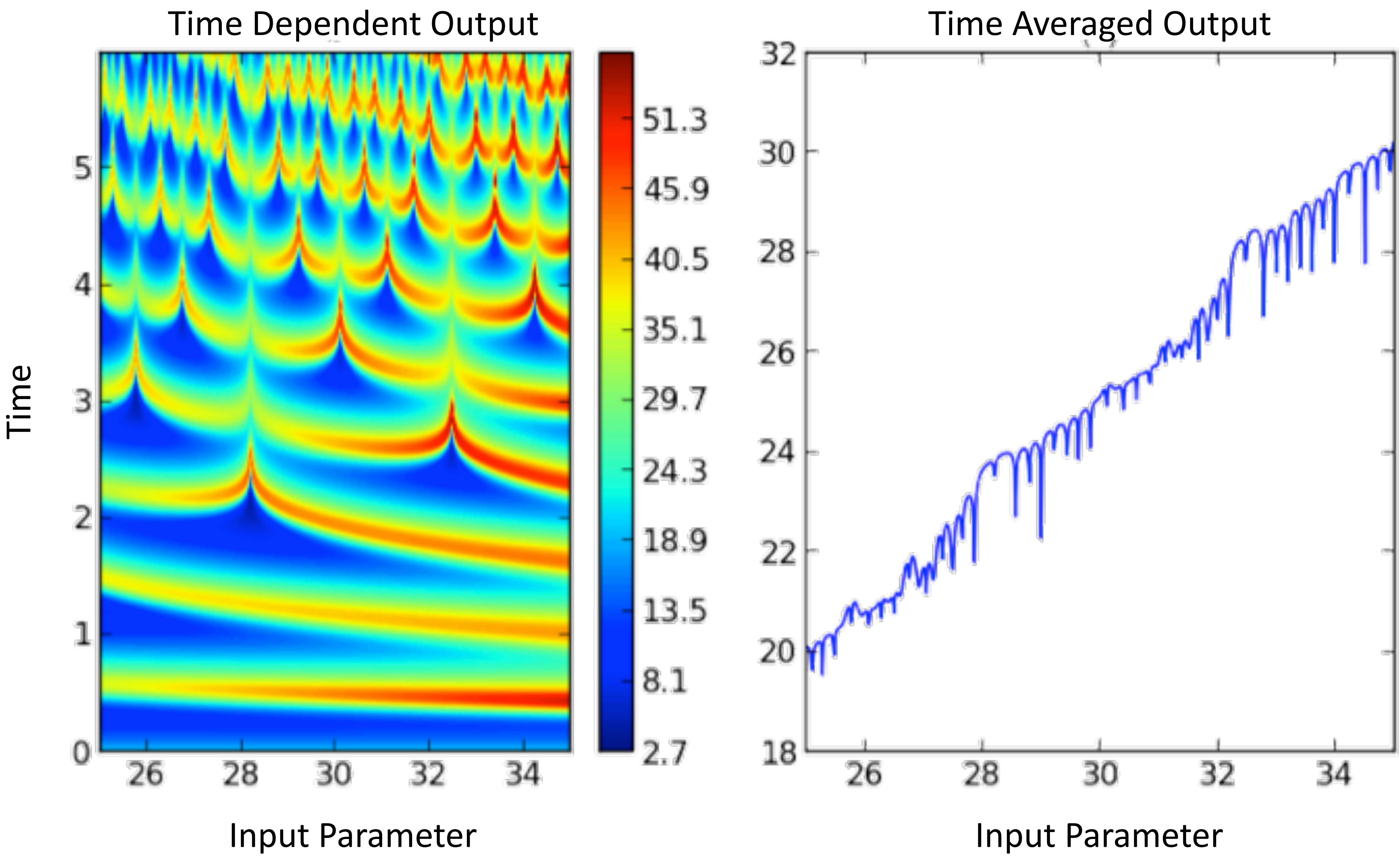




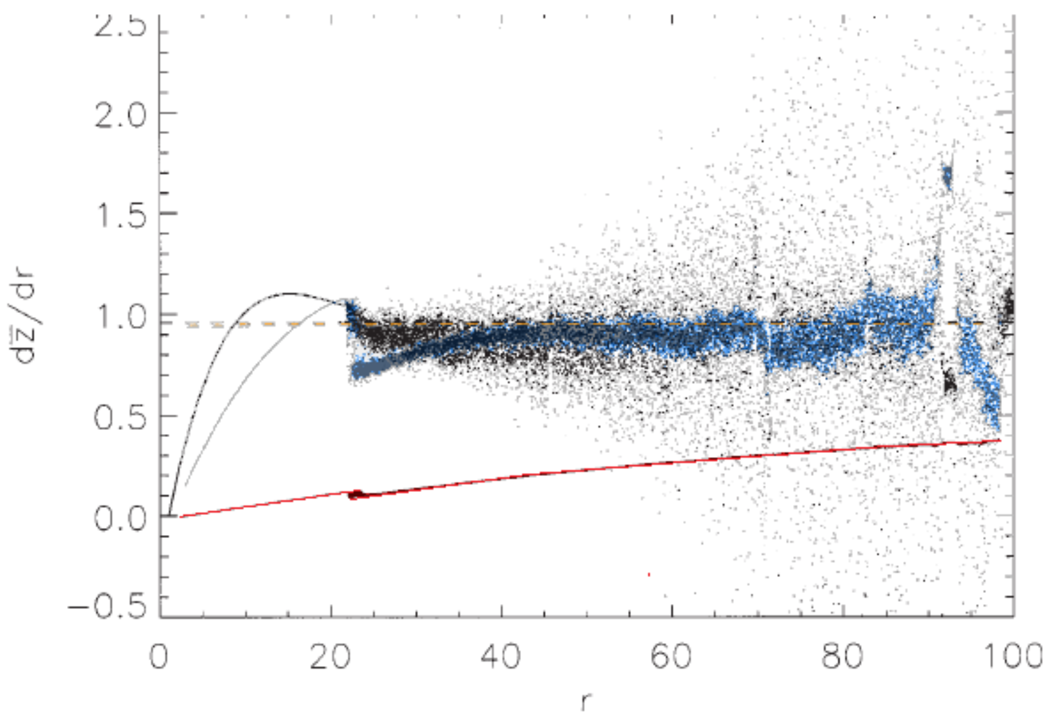


- **Lorenz 63 System**
- Objective z: rate of heat transfer
- Input ρ: temperature difference

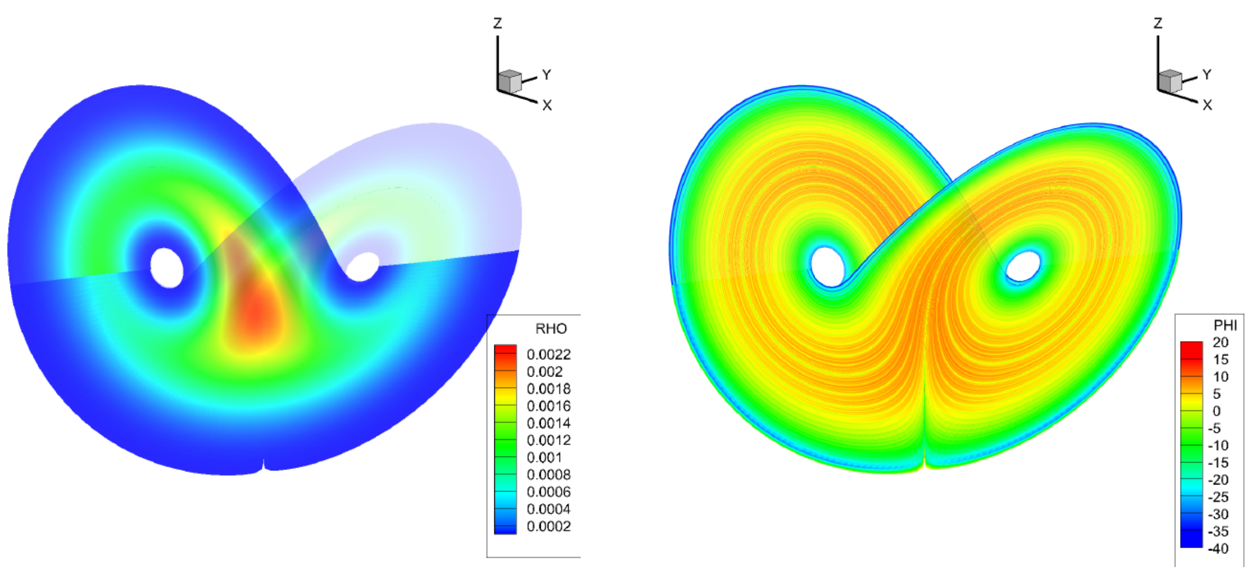
Failure of conventional sensitivity analysis for chaos



Sensitivity analysis approaches for chaotic systems

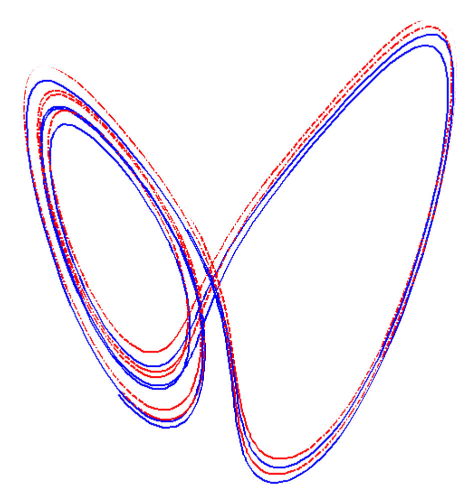


1. Ensemble adjoint sensitivities for short, medium, and long time segments.



2. Fokker-Planck computed stationary density (left) and its adjoint (right).

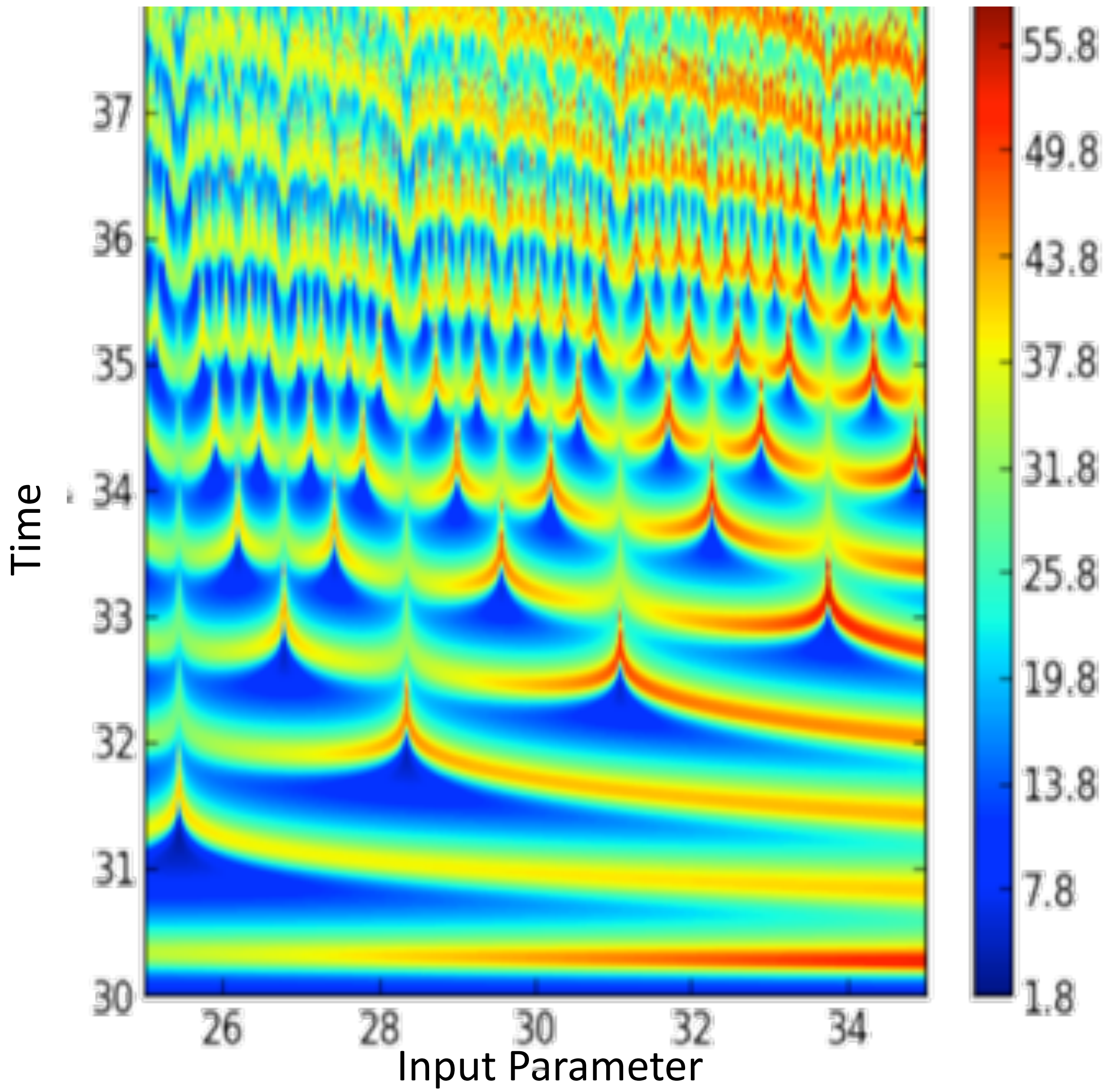
1. Ensemble Adjoint Method
   - Lea et al. 2000, Eyink et al. 2004.
2. Fokker-Planck Methods
   - Thuburn et al. 2005., Blonigan and Wang 2014
3. Fluctuation-Dissipation Theorem
   - Leith 1975, Abramov and Majda 2007
4. **Least Squares Shadowing (LSS)**
   - Wang, Hui, and Blonigan 2014



4. LSS reference and shadow trajectories.

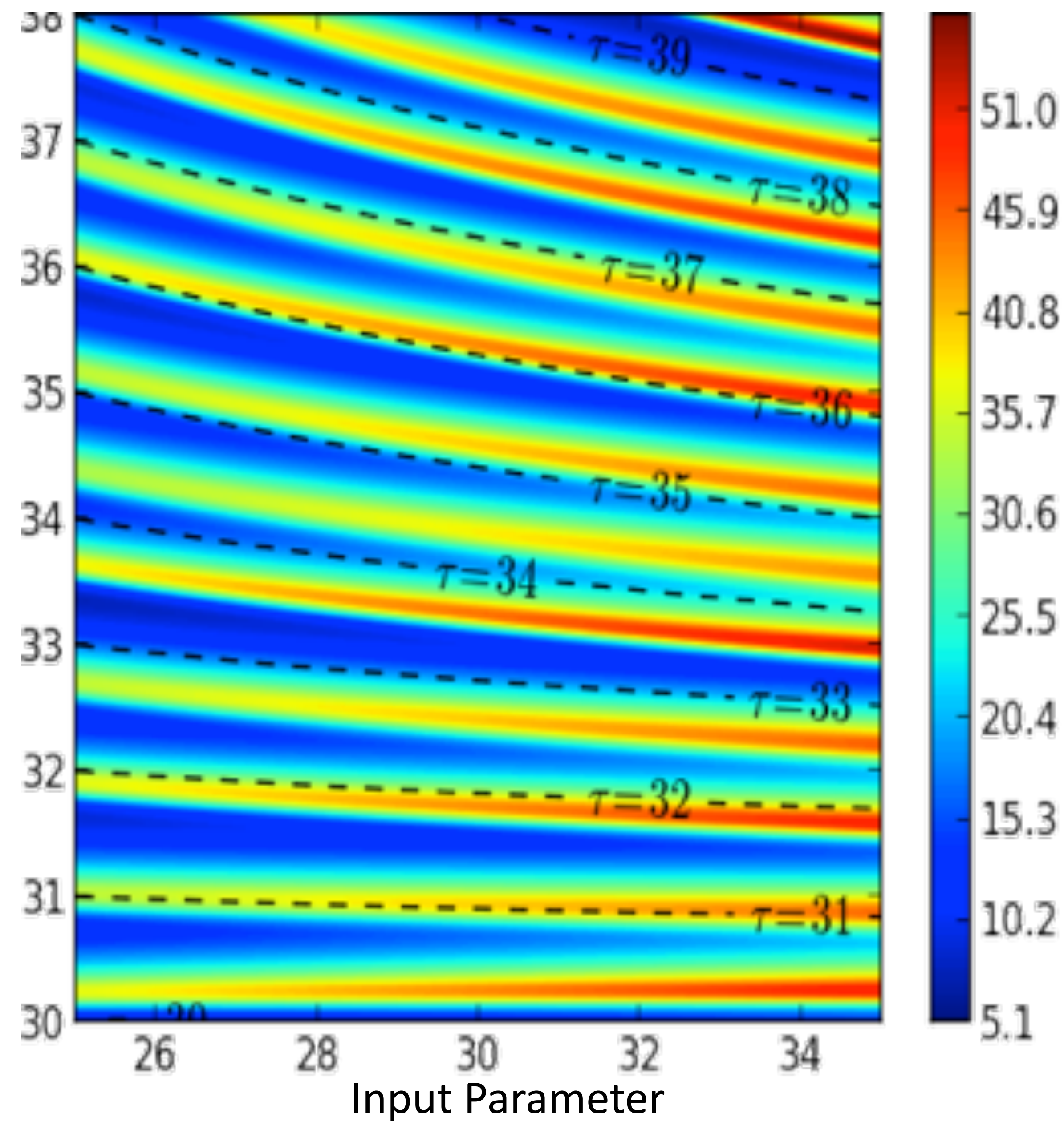
Sensitivity analysis with shadowing

Conventional Objective Surface



- Fixed initial condition for all input parameter values.

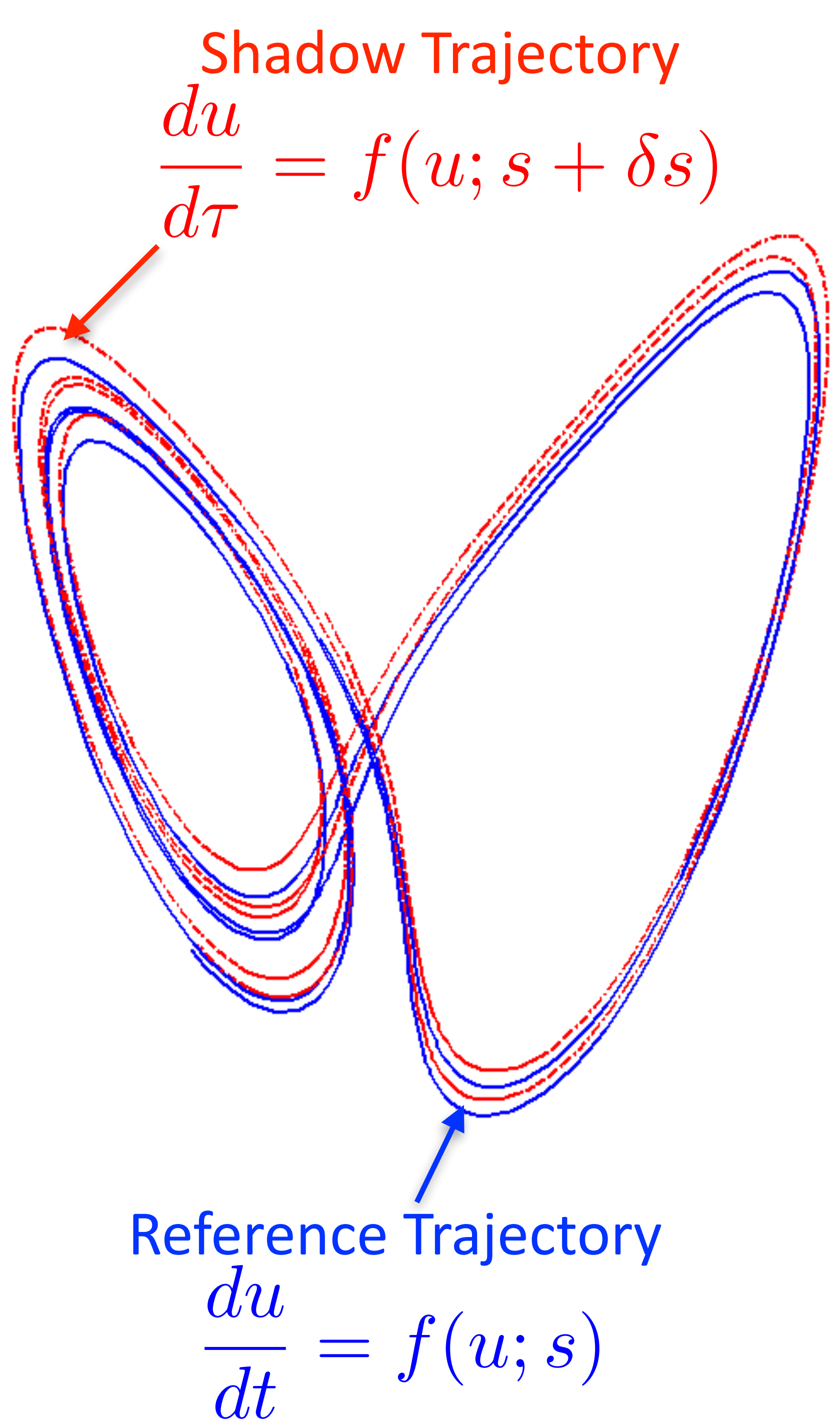
Shadowing Objective Surface



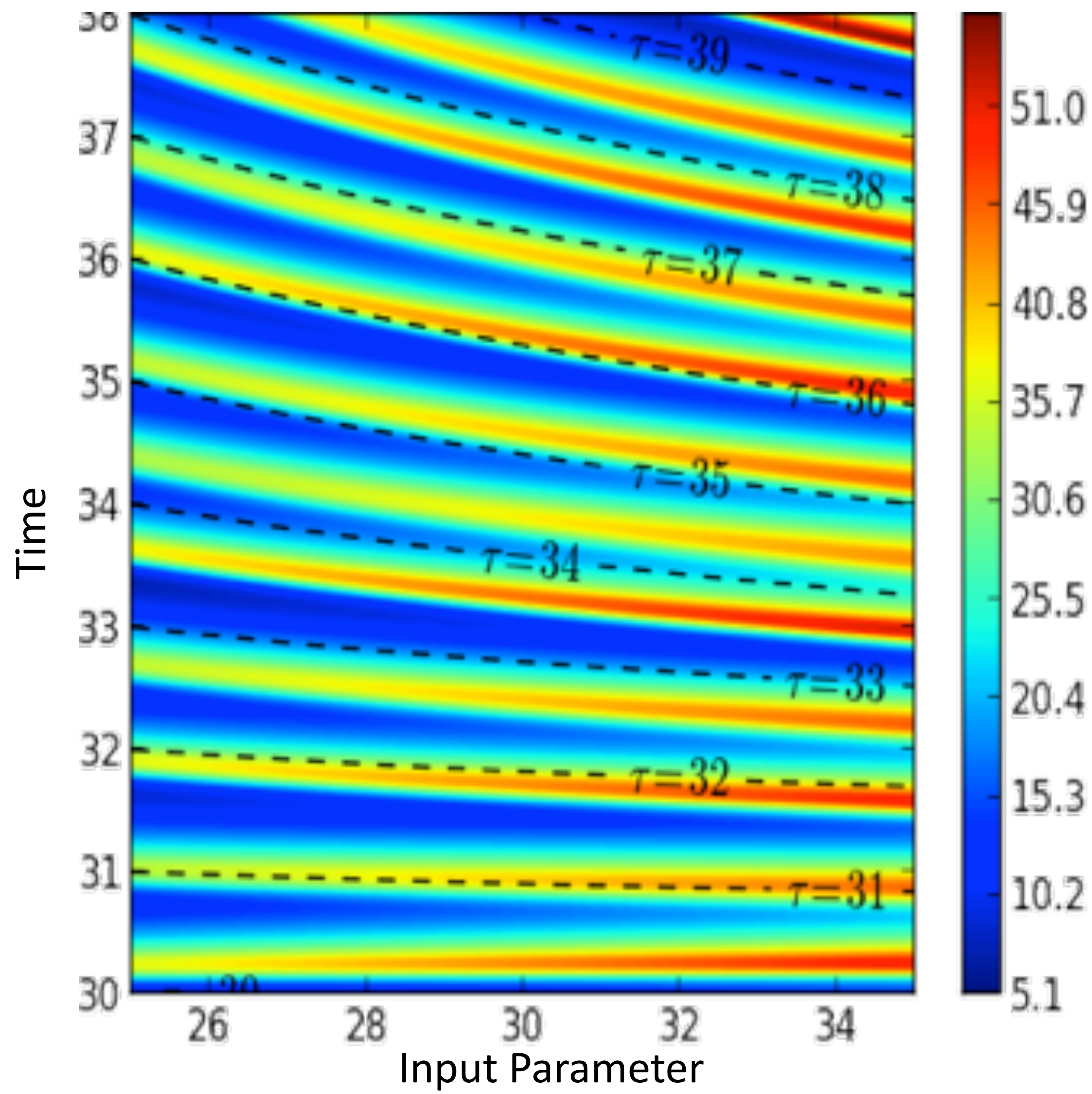
- Choose initial condition for smooth variation of objective history with input parameter.

Sensitivity analysis with shadowing

In Phase Space:



Shadowing Objective Surface



- Choose initial condition for smooth variation of objective history with input parameter.

Least squares shadowing

- Assume ergodicity, replace initial condition for u(t) with

$$\min_{u,\tau} \frac{1}{2} \int_{T_0}^{T_1} W(t) \| u(\tau(t)) - u_r(t) \|^2 \, dt$$

$$\text{s.t.} \quad \frac{du}{d\tau} = f(u; s + \delta s)$$

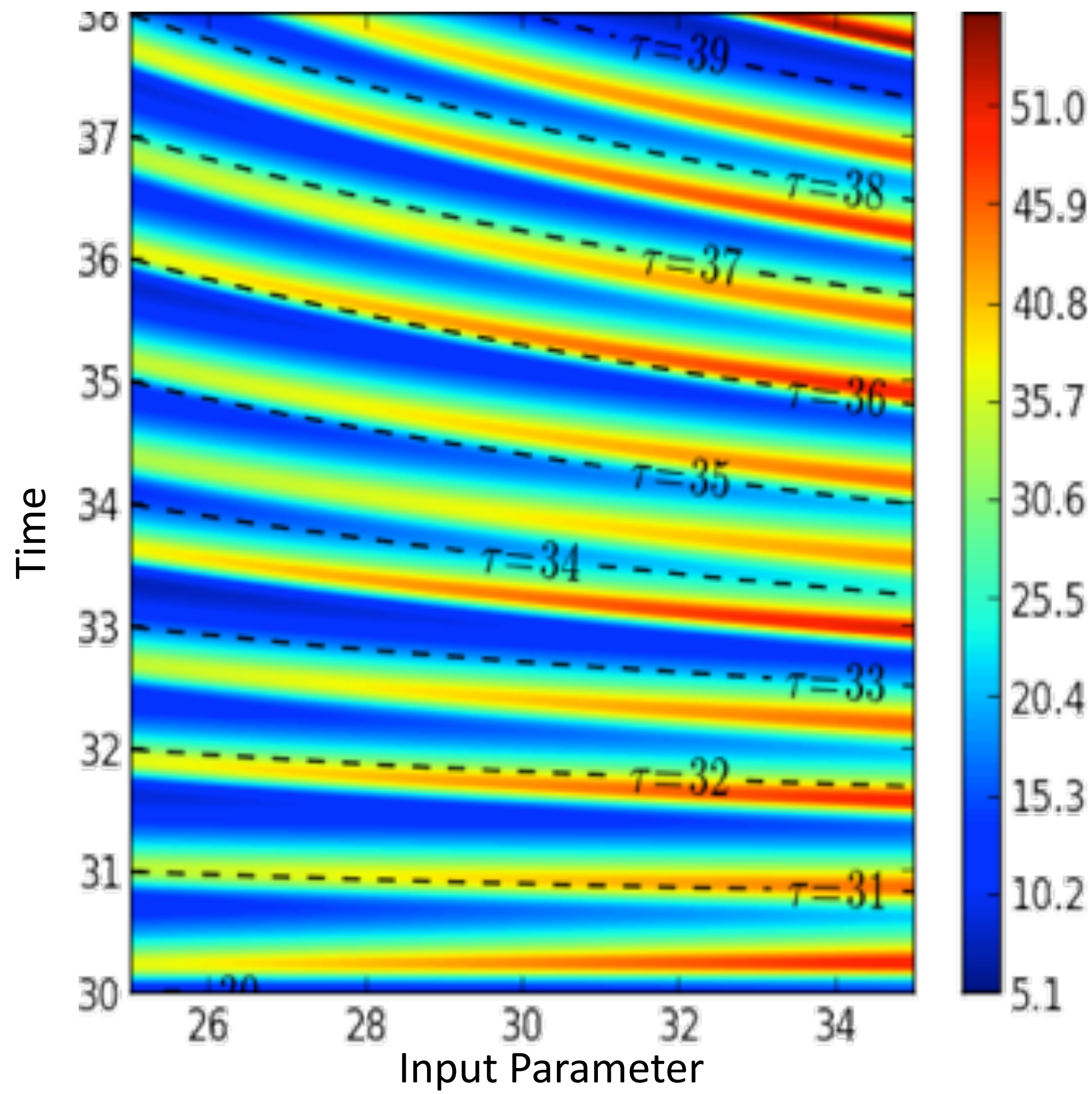
Linearize for tangent LSS:

$$v \equiv \frac{\partial u}{\partial s} \Rightarrow \min_{v} \frac{1}{2} \int_{T_0}^{T_1} W(t) \| v(t) \|^2 \, dt$$

$$\text{s.t.} \quad \frac{dv}{dt} = \frac{\partial f}{\partial u} v + \frac{\partial f}{\partial s} + \underbrace{\left(1 - \frac{d\tau}{dt}\right)}_{\eta} f$$

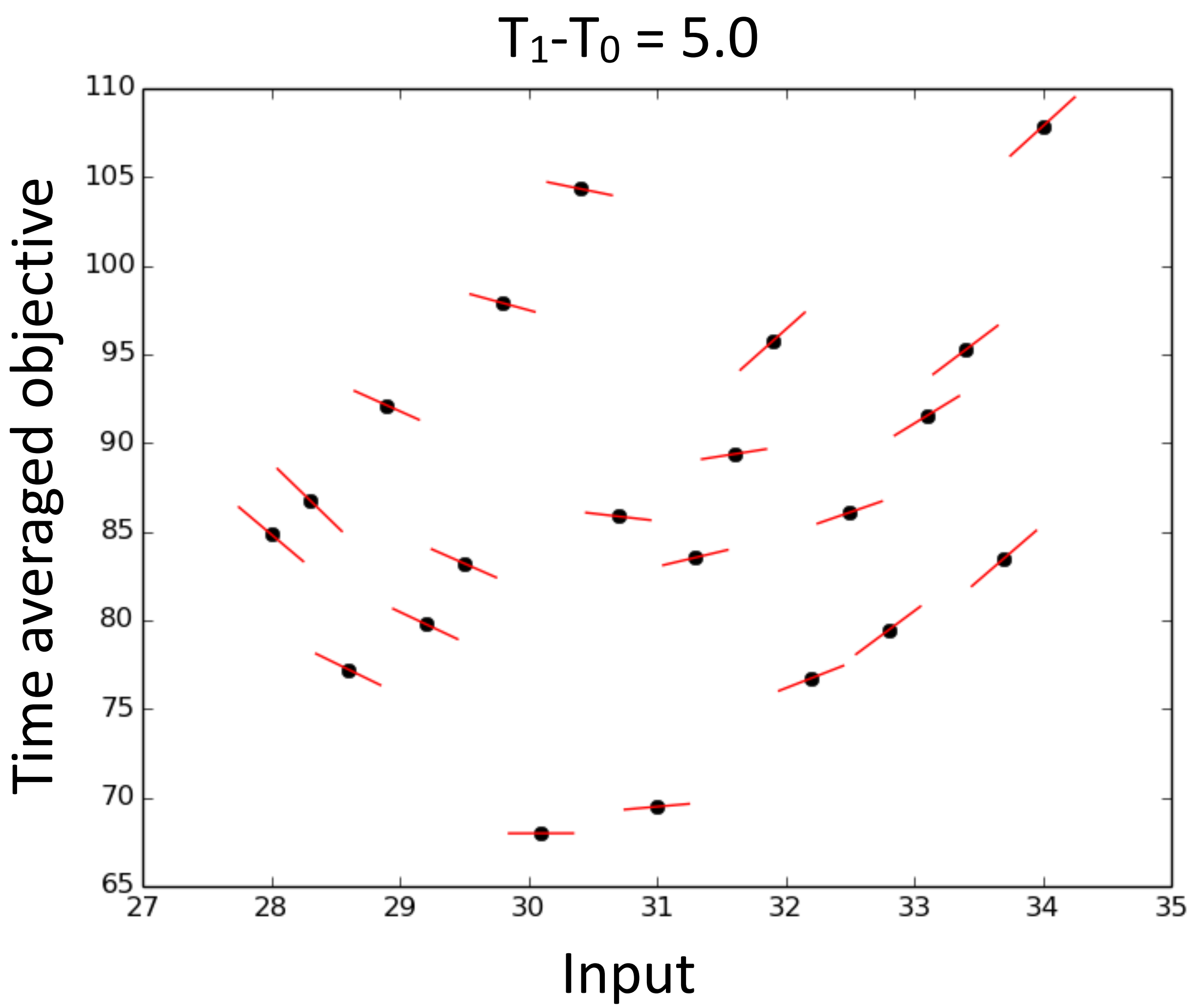
$$\text{s.t.} \quad \left\langle v, \frac{du}{dt} \right\rangle = 0$$

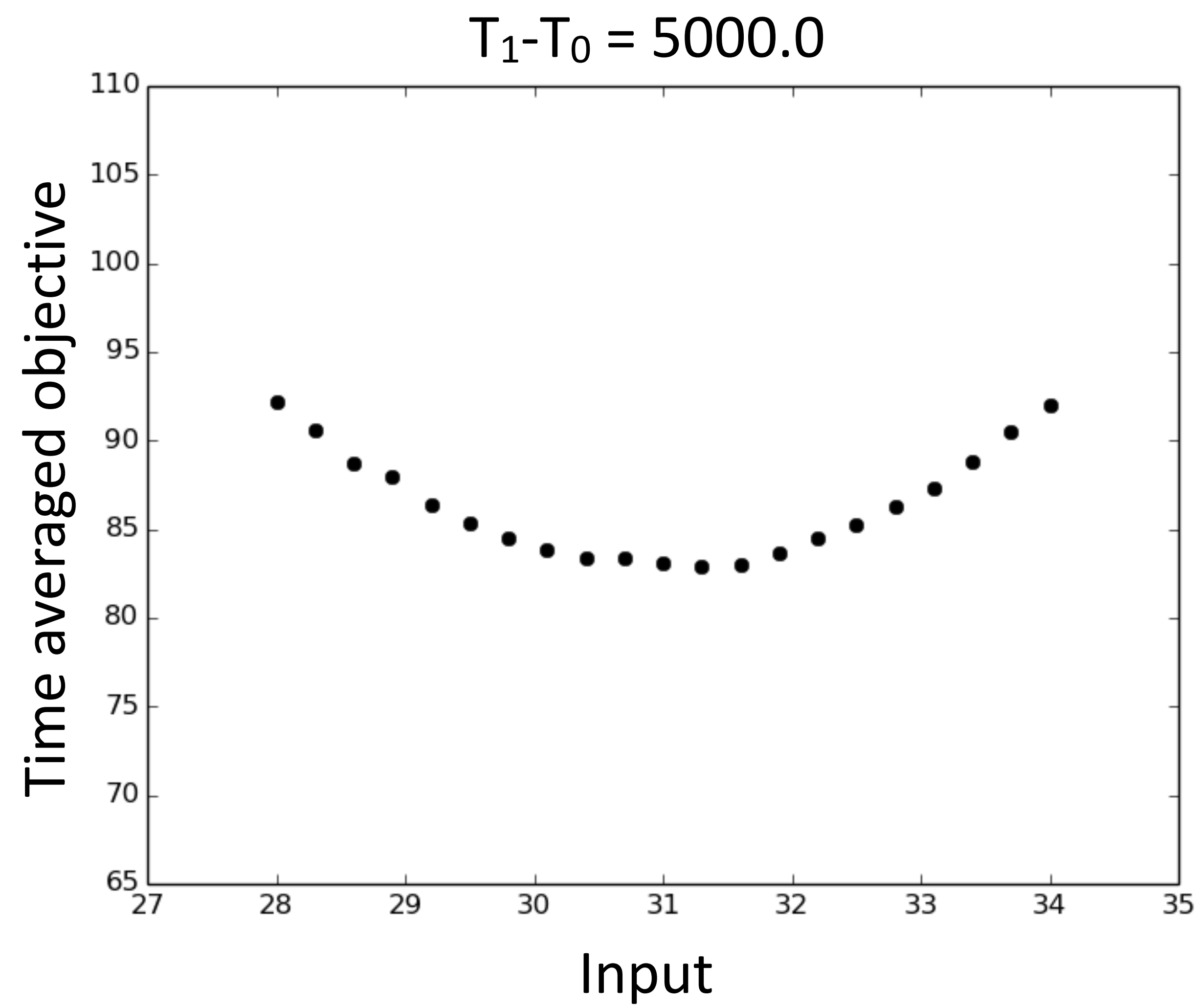
Shadowing Objective Surface

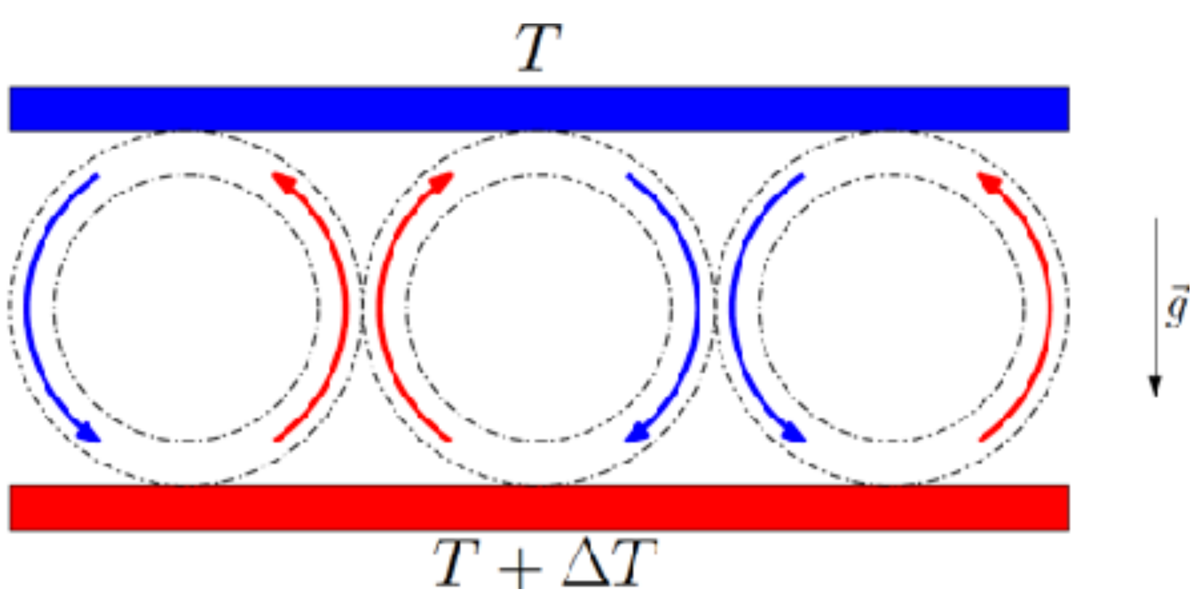


- Choose initial condition for smooth variation of objective history with input parameter.

Least squares shadowing for Lorenz 63







- **Lorenz 63 System**
- Objective (z-28): deviation of rate of heat transfer
- Input ρ: temperature difference

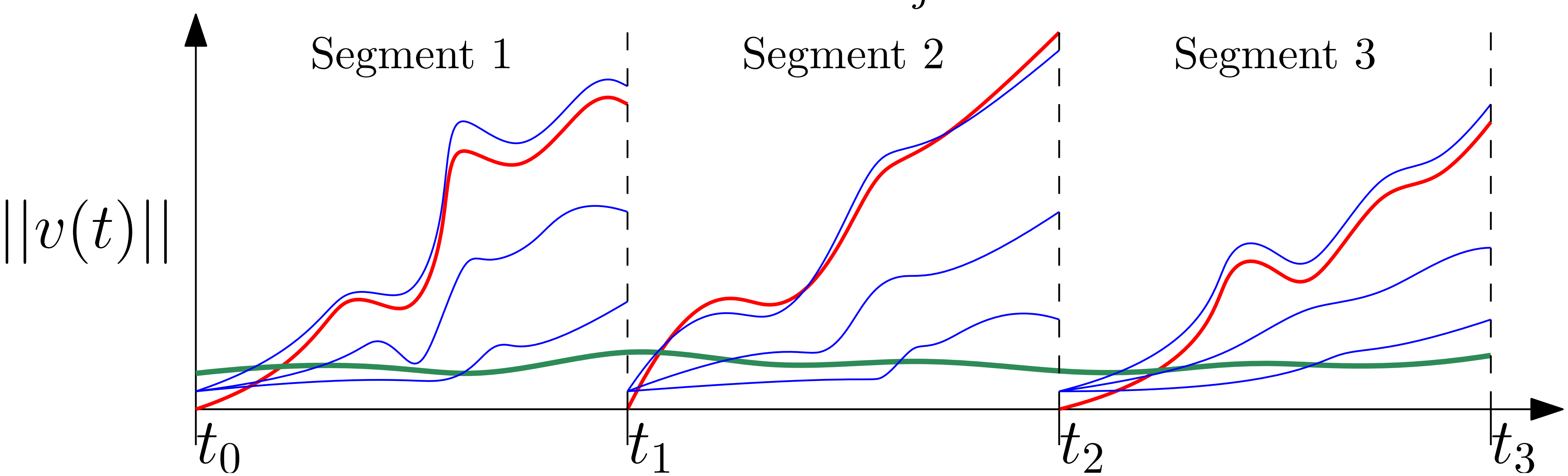
"Non-Intrusive" least squares shadowing

- Originally proposed by Ni et al. (AIAA 2016-4399)
- Reduces size of LSS minimization problem considerably by
  - Minimizing v(t) at K discrete checkpoints in time

$$\min_{v(t_i)} \frac{1}{2} \sum_{i=0}^{K} \|v(t_i)\|^2 \quad \text{s.t.} \quad \frac{dv}{dt} = \frac{\partial f}{\partial u} v + \frac{\partial f}{\partial s} + \eta f, \quad \left\langle v, \frac{du}{dt} \right\rangle = 0$$

  - Expressing v(t) in terms of homogeneous and inhomogeneous components

$$v(t) = \sum_j \alpha_j \tilde{v}_j(t) + \hat{v}(t)$$



Homogeneous

$$\frac{d\tilde{v}_j}{dt} = \frac{\partial f}{\partial u} \tilde{v}_j,$$

$$\tilde{v}_j(t_i) = V_i^j$$

Inhomogeneous

$$\frac{d\hat{v}}{dt} = \frac{\partial f}{\partial u} \hat{v} + \frac{\partial f}{\partial s} + \eta f,$$

$$\hat{v}(t_i) = \hat{V}_i$$

→ **Choose α that solves the least squares problem**

Tangent NILSS Algorithm

- Set $\hat{V}_0 = 0$ and $V_0 = \mathcal{Q}_0$, a random orthonormal matrix.
- For each segment starting with 1:
  1. Compute primal $u(t)$ from t_{i-1} to t_i
  2. Compute all m $\tilde{v}_j(t)$ from $\tilde{v}_j(t_{i-1}) = V_{i-1}^j$
  3. Compute QR-decomposition $\mathcal{Q}_i \mathcal{R}_i = V_i^-$, where $[V_i^-]^j = \tilde{v}_j(t_i)$
  4. Set $V_i^j = \mathcal{Q}_i^j$
  5. Compute $\hat{v}(t)$ for $\hat{v}(t_{i-1}) = \hat{V}_i$ with $\hat{V}_i = (\mathcal{I} - \mathcal{Q}_{i-1}\mathcal{Q}_{i-1}^T)\hat{v}(t_{i-1}^-)$
- Solve

$$\min \left\| \begin{matrix} \alpha_1 \\ \vdots \\ \alpha_K \\ \alpha_{K+1} \end{matrix} \right\|_2 \quad \text{s.t.} \quad \begin{bmatrix} \mathcal{R}_1 & -\mathcal{I} & & \\ & \ddots & \ddots & \\ & & \mathcal{R}_K & -\mathcal{I} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_K \\ \alpha_{K+1} \end{bmatrix} = \begin{bmatrix} -\mathcal{Q}_1^T \hat{v}(t_1^-) \\ \vdots \\ -\mathcal{Q}_K^T \hat{v}(t_K^-) \end{bmatrix}$$

- Compute sensitivity to s with α_i's and segment sensitivity contributions g_i and h_i

$$\frac{d\bar{J}}{ds} = \frac{1}{t_K - t_0} \sum_{i=1}^{K} \left({g_i}^T \alpha_i + h_i \right) + \frac{\partial \bar{J}}{\partial s}$$

Adjoint NILSS Algorithm

- Set $V_0 = \mathcal{Q}_0$, a random orthonormal matrix.
- For each segment starting with 1:
  1. Compute primal $u(t)$ from t_{i-1} to t_i
  2. Compute all m $\tilde{v}_j(t)$ from $\tilde{v}_j(t_{i-1}) = V_{i-1}^j$
  3. Compute QR-decomposition $\mathcal{Q}_i\mathcal{R}_i = V_i^-$, where $[V_i^-]^j = \tilde{v}_j(t_i)$
  4. Set $V_i^j = \mathcal{Q}_i^j$
- Solve the minimization problem

$$\min \left\| \begin{bmatrix} \mathcal{R}_1^T & & \\ -\mathcal{I} & \ddots & \\ & \ddots & \mathcal{R}_K^T \\ & & -\mathcal{I} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \vdots \\ \psi_K \end{bmatrix} - \begin{bmatrix} g_1 \\ \vdots \\ g_K \end{bmatrix} \right\|_2$$

- Set $w(t_K^+) = 0$. For each segment starting with K solve the adjoint equation backwards from t_i to t_{i-1}, where the matrix P_{t_i} and vector x_i are related to τ(t).

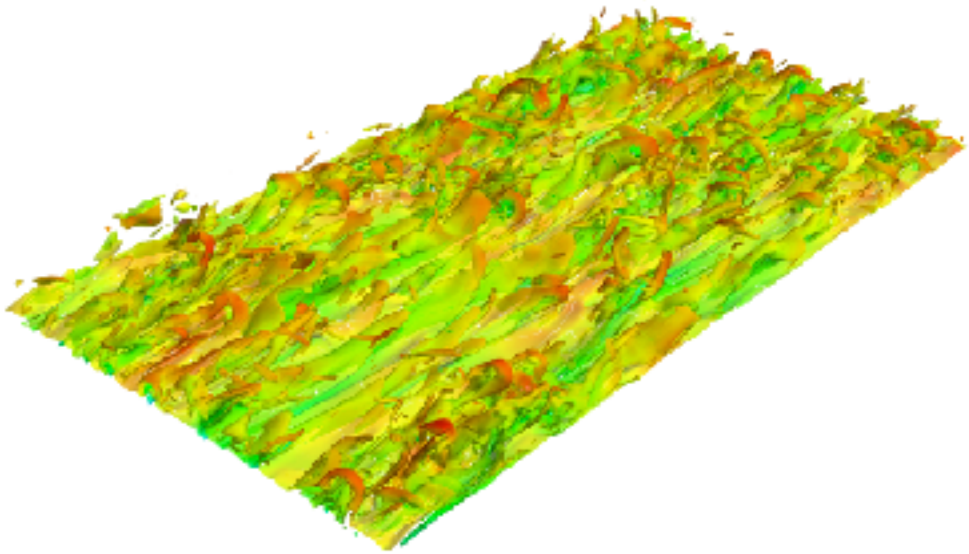
$$-\frac{dw}{dt} = \left[\frac{\partial f}{\partial u}\right]^T w + \frac{1}{t_K - t_0}\frac{\partial J}{\partial u} \qquad w(t_i^-) = P_{t_i}\left((\mathcal{I} - \mathcal{Q}_i\mathcal{Q}_i^T)w(t_i^+) - \mathcal{Q}_i\psi_i\right) + x_i$$

- Compute sensitivities with

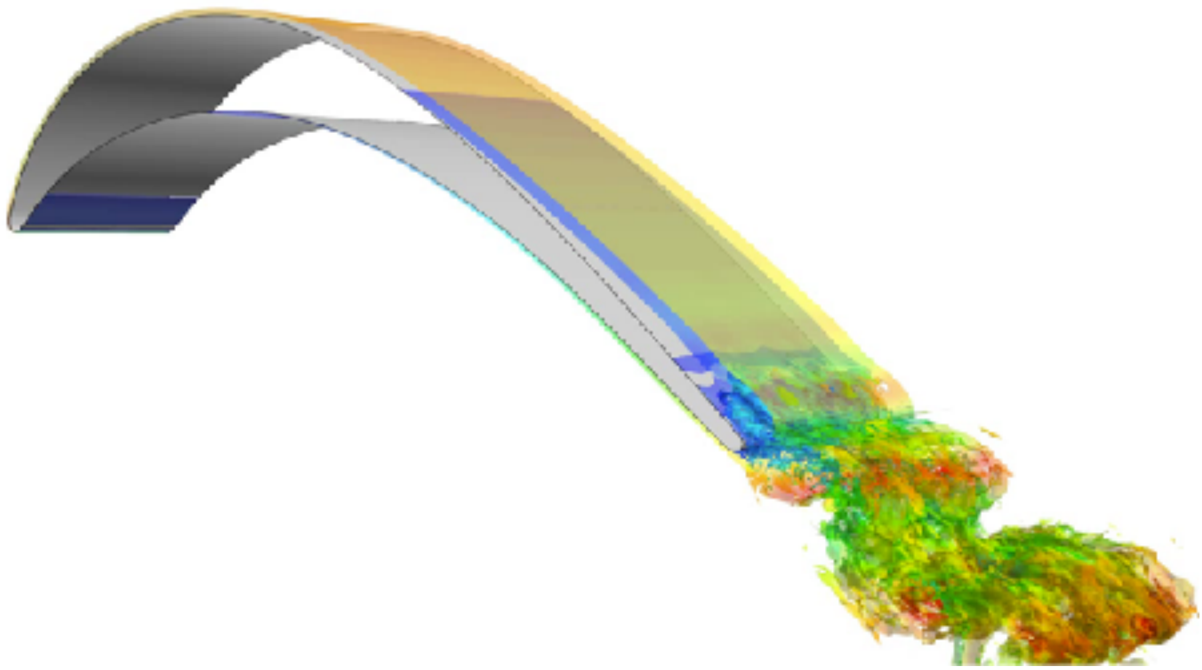
$$\frac{d\bar{J}}{ds} = \int_{t_0}^{t_K} \left.\frac{\partial f}{\partial s}\right|_t w(t)\ dt + \frac{\partial \bar{J}}{\partial s}$$

NILSS computational cost

- 1 cost unit = primal solution for a single segment
- **Cost of Adjoint NILSS: ~(m+3)K units**
  - Primal on K segments costs K units
  - m tangent solutions cost ~mK units
  - K QR-decompositions:
    - Parallel TSQR: $2N_{DOF}m^2/P + 2m^3/3$ flops
  - Minimization Problem
    - Usually a relatively small cost
  - Adjoint on K segments costs ~2K units
    - File I/O could drive compute time
- m is at least the number of positive Lyapunov exponents.
  - Re_τ=180 channel flow, m ≈ 1,500
  - T106C turbine blade, m ≈ 400



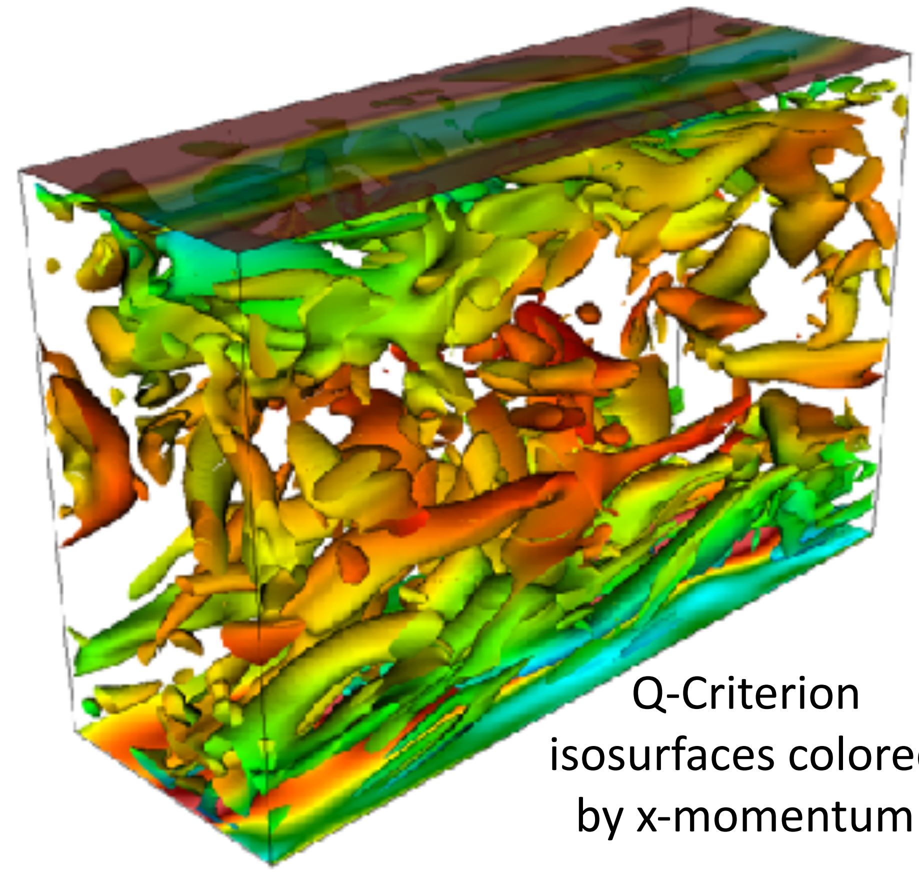
Channel flow: Vorticity magnitude isosurfaces colored by streamwise velocity



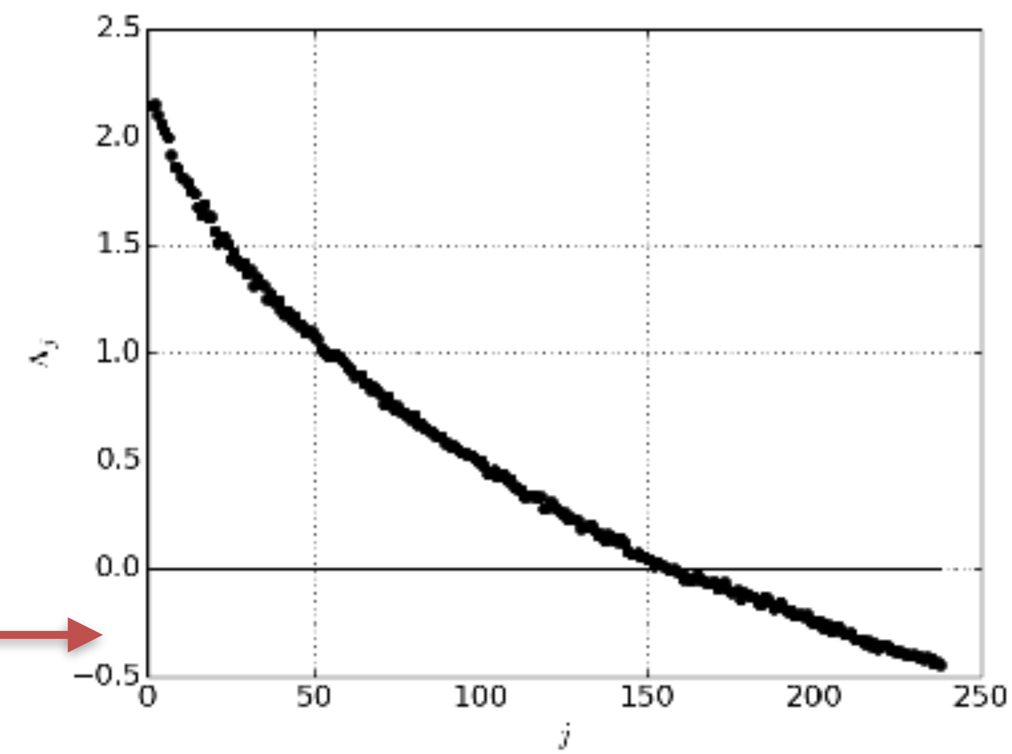
Turbine blade: Vorticity magnitude isocontours colored by mach number

Minimum Turbulent Flow Unit

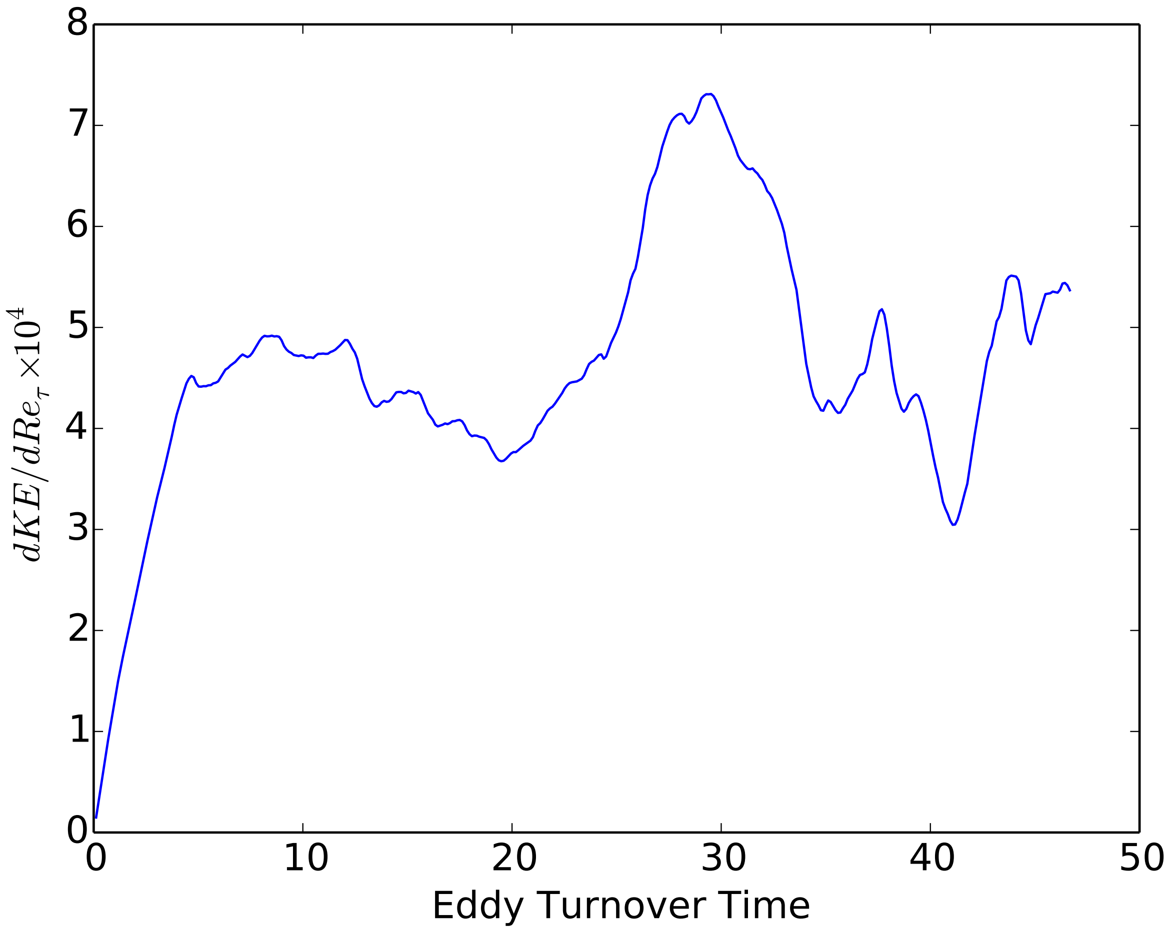
- Smallest channel that can sustain turbulent flow (Jimenez and Moin, 1991).
  - Very good agreement with turbulent channel statistics below $y^+=40$
- Current study replicates a case in the original paper
  - $Re=3000$, $Re_\tau=140$
  - Channel size=$\pi h \times 2h \times 0.34\pi h$
- Flow Solver: eddy
  - Discontinuous Galerkin Spectral Element Method (DGSEM) framework
  - Space-time DG discretization
  - Entropy stable flux of Ismail and Roe
- Mesh: 32x128x16 Degrees of Freedom
- Roughly 150 positive Lyapunov exponents

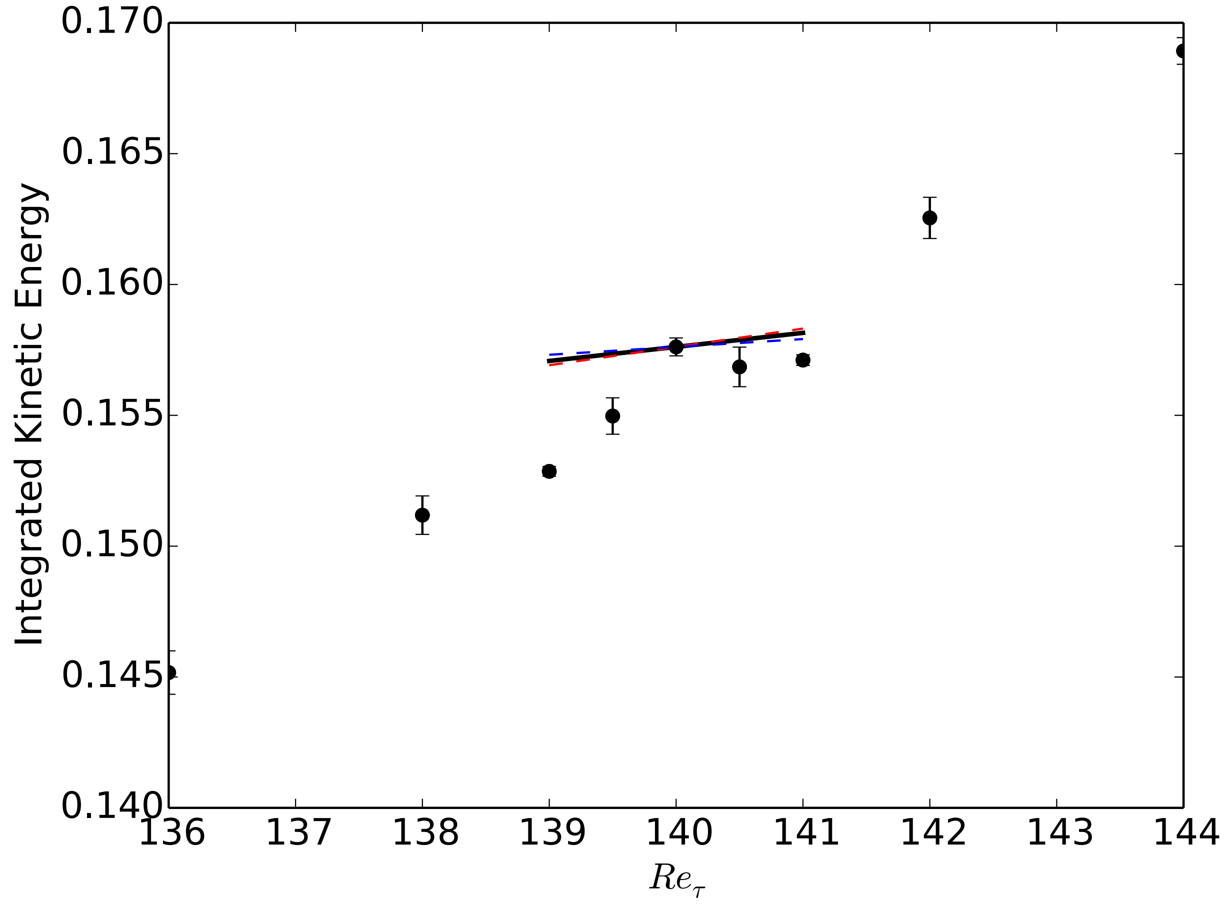


Q-Criterion isosurfaces colored by x-momentum



NI-LSS Sensitivity



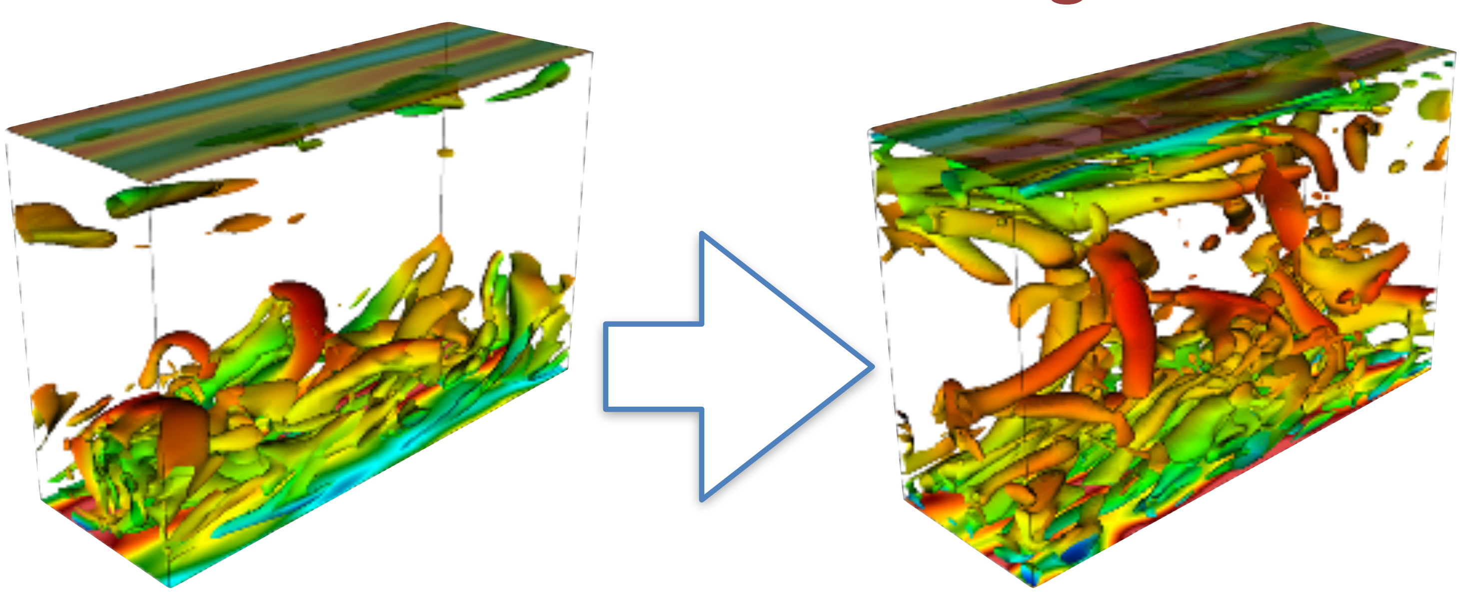


- NI-LSS run with 160 modes
- Objective function is volume-integrated kinetic energy
- Sensitivity to Re_τ computed
- Slow convergence of sensitivity due to long time scales present in flow unit

NI-LSS Adjoint

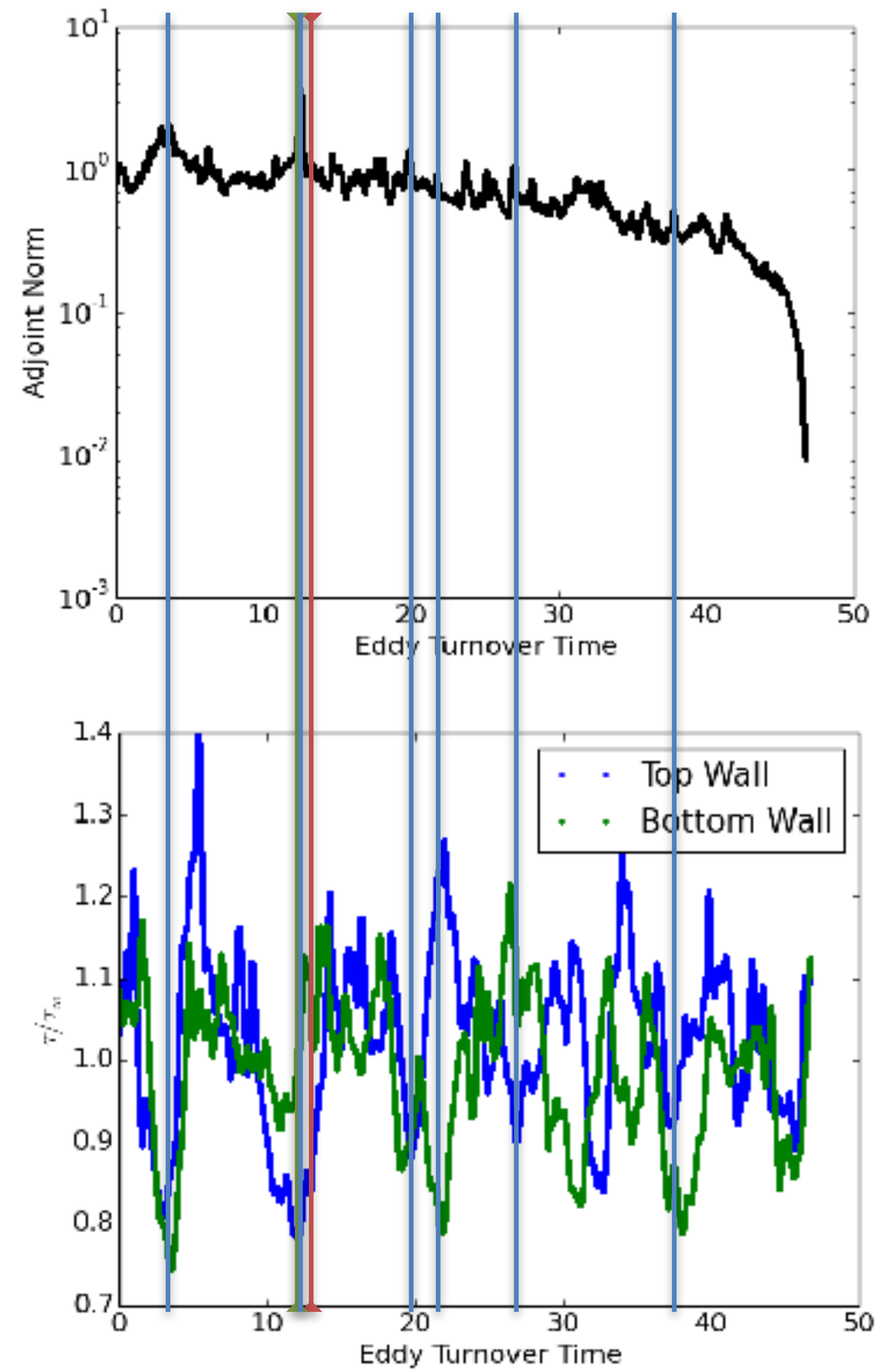
- Shadowing adjoint does not exhibit exponential growth
- Adjoint provides physical insights
  - Largest adjoint magnitudes occur before “blooming” of turbulence indicated by wall shear stress τ.

Turbulence “Blooming”



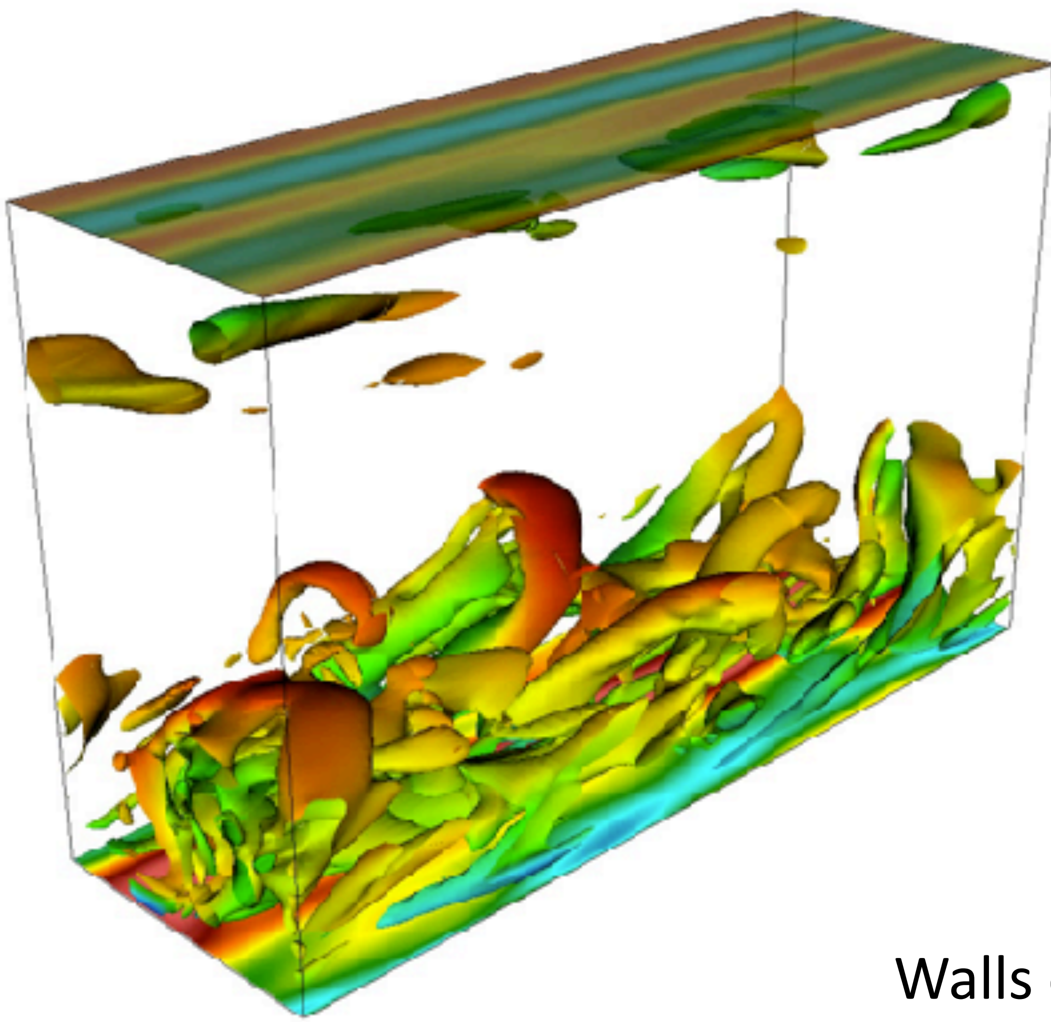
t=12.13 t=13.18

Q-Criterion isosurfaces colored by x-momentum

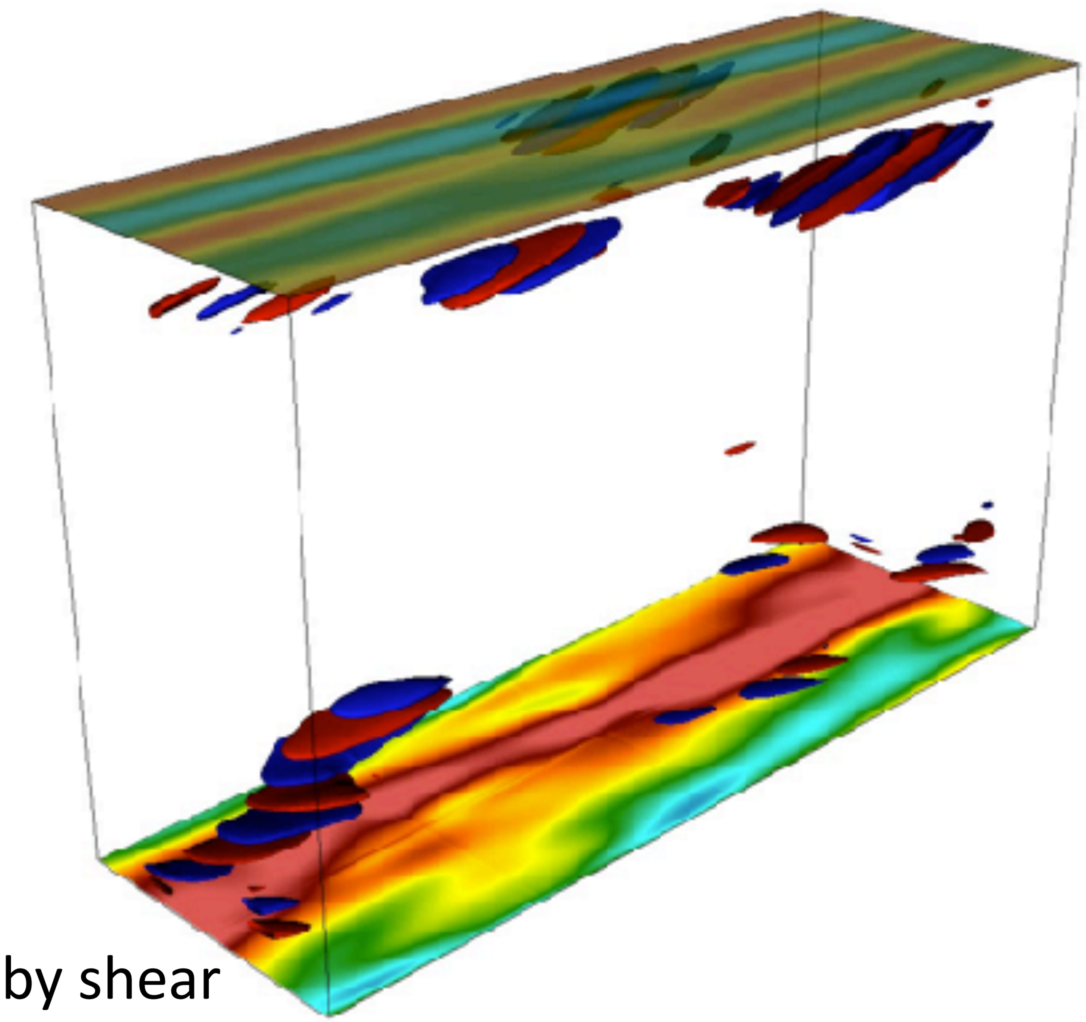


Flow Unit Adjoint Field

Q-Criterion isosurfaces colored by x-momentum



Adjoint X-momentum isocontours for ±2.0

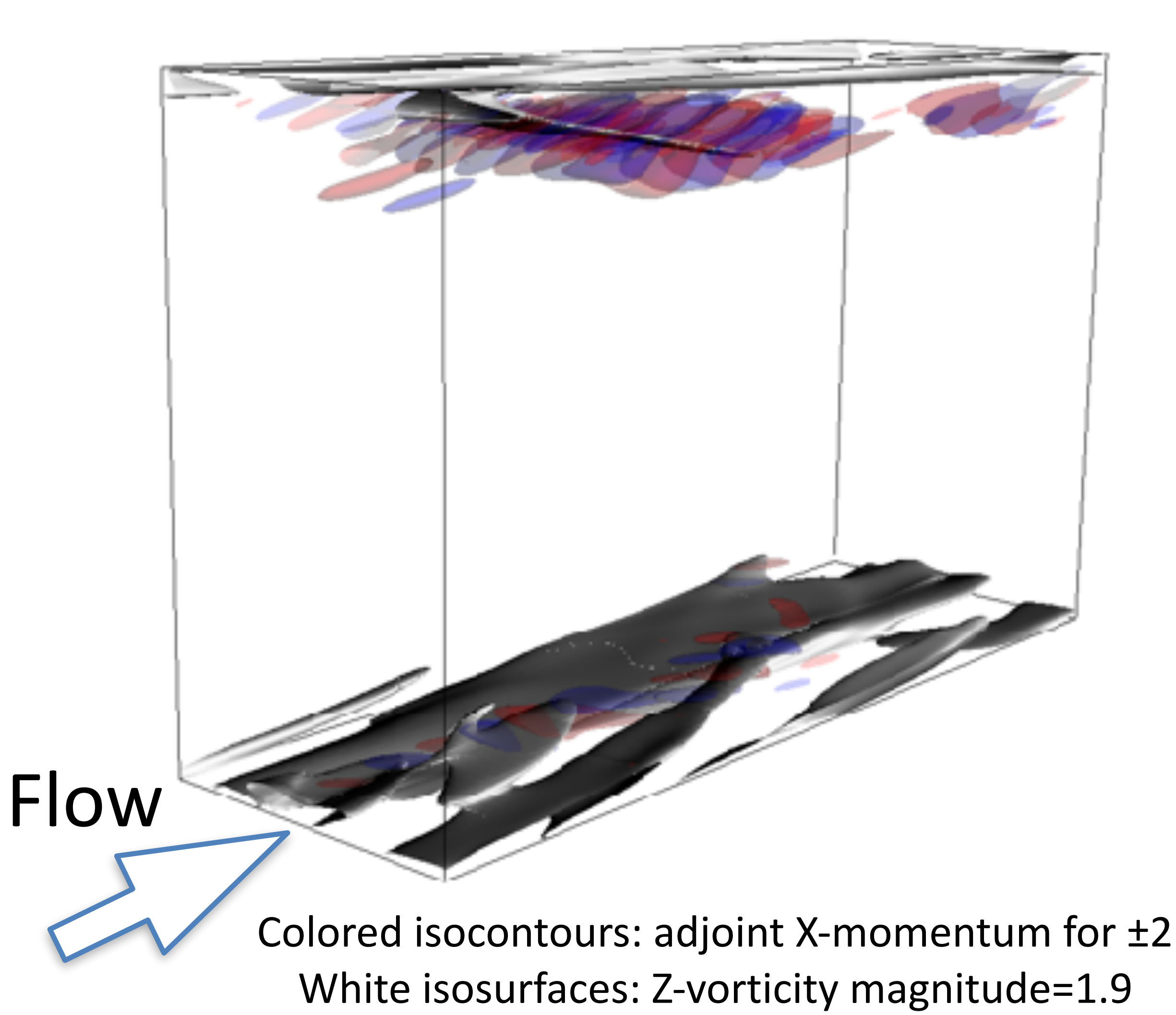


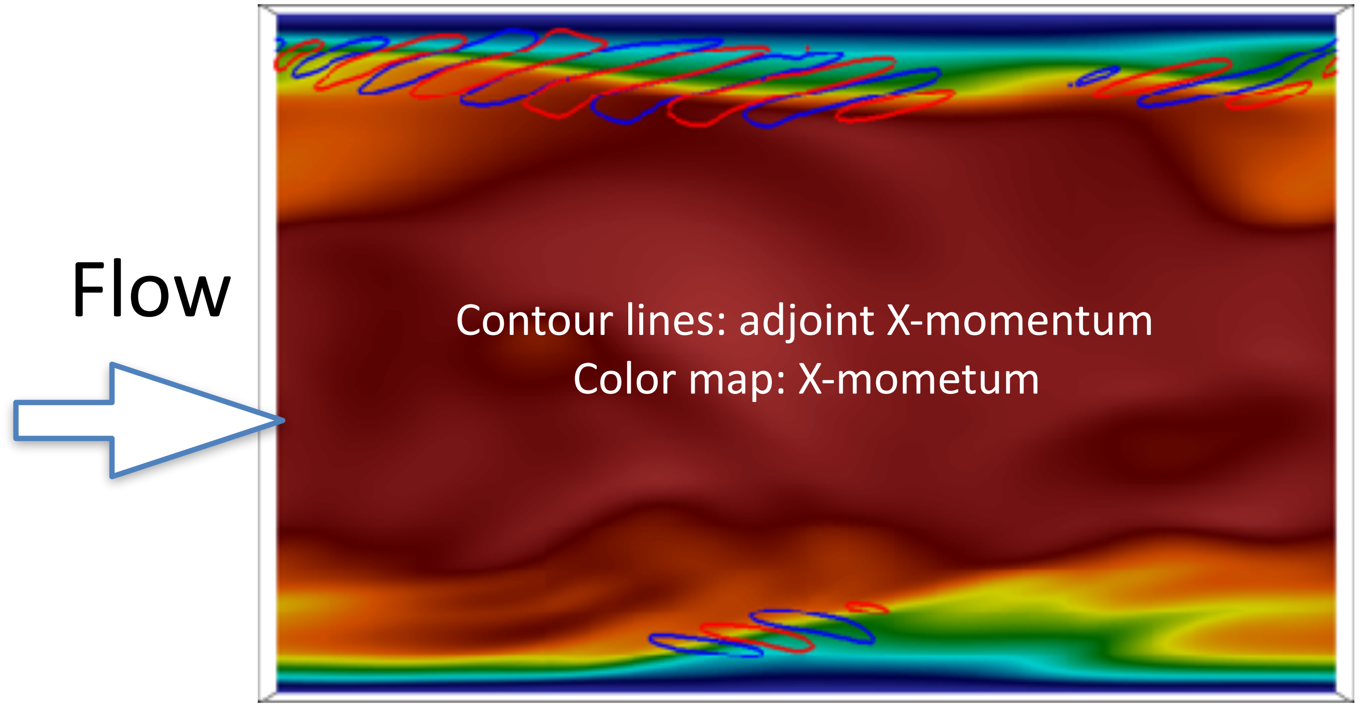
Walls colored by shear force Magnitude

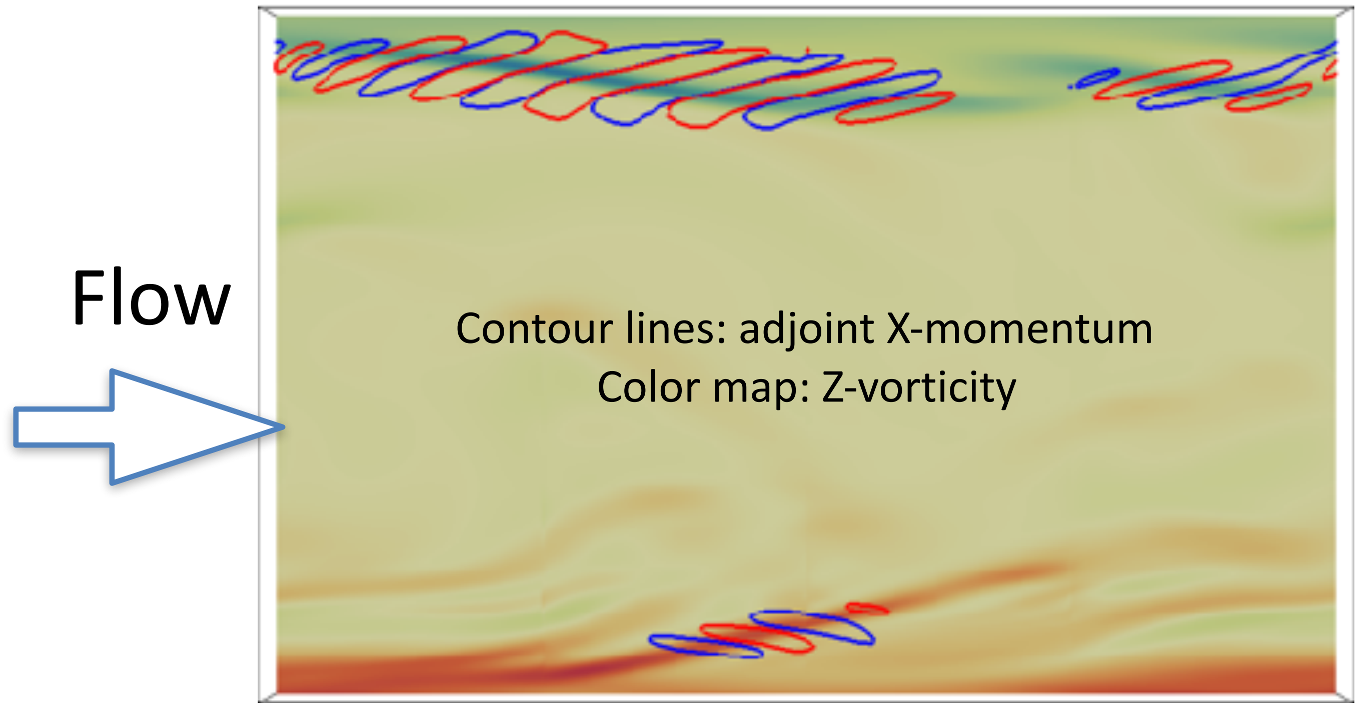
- Integrated kinetic energy adjoint shows when and where flow is most susceptible to flow instabilities

Adjoint Field and Z-vorticity

Snapshots from t=12.13



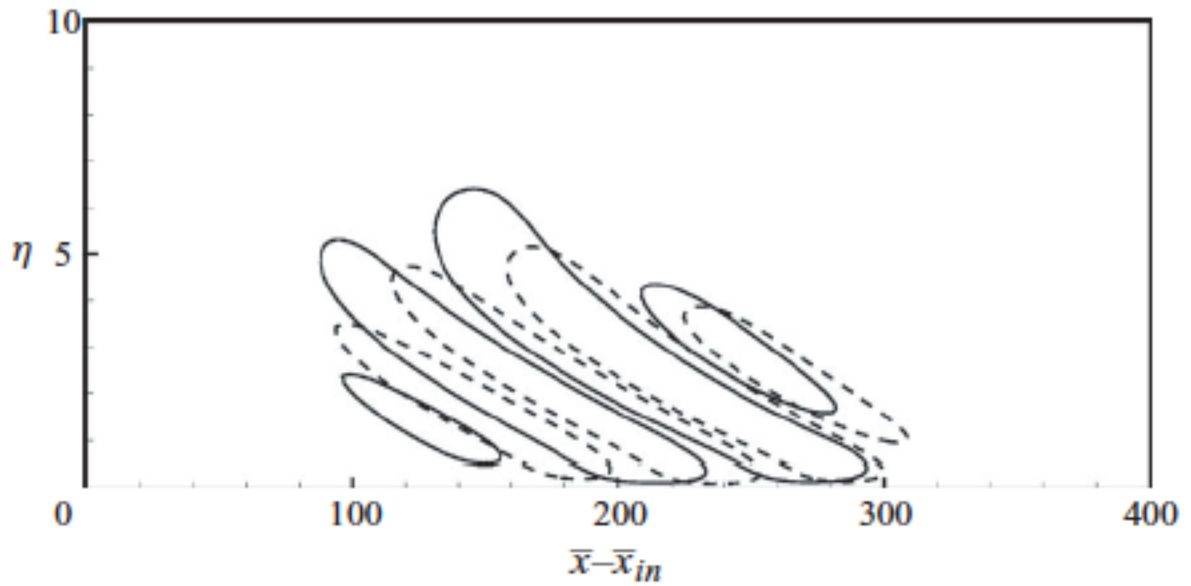




- Time-averaged, volume-integrated kinetic energy is sensitive to perturbations in the sheets of Z-vorticity being transported away from the walls.

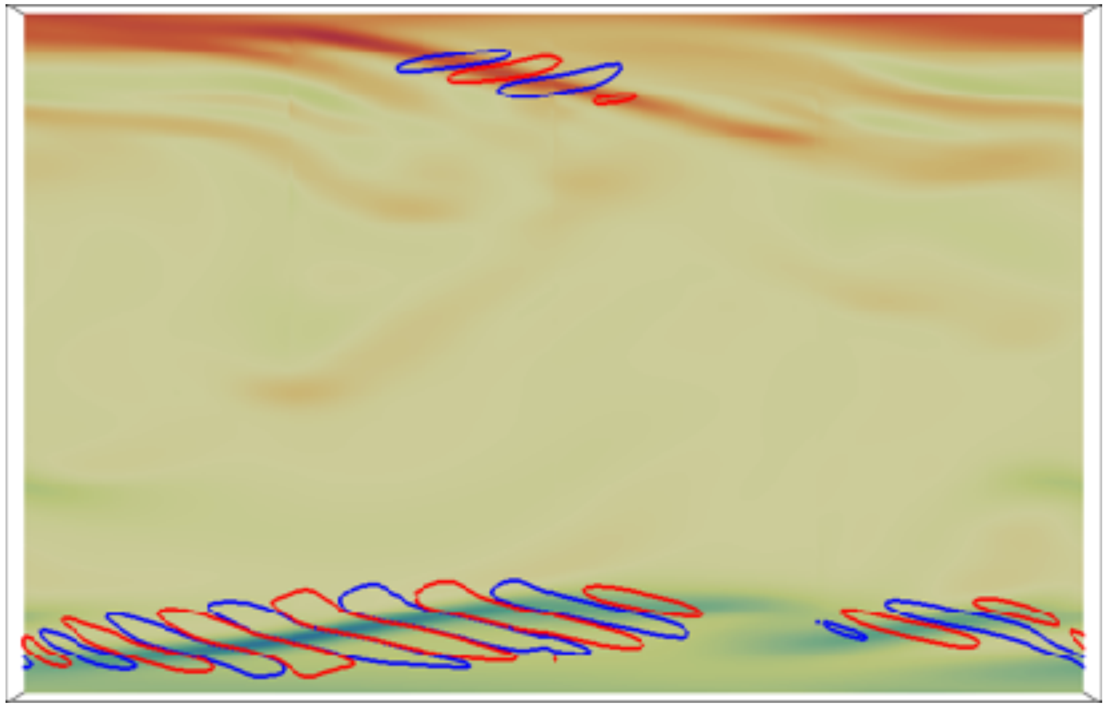
Optimal Perturbation for Transition

- Streamwise velocity magnitude contours for a flow perturbation optimized to increase the kinetic energy of Re=610 flow over a flat plate (Cherubini et al. 2010, JFM):



Solid lines: domain length = 400 units
Dotted lines: domain length = 800 units

- Adjoint X-momentum field for flow unit prior to turbulence "blooming":



Contour lines: X-momentum adjoint
Color map: Z-vorticity

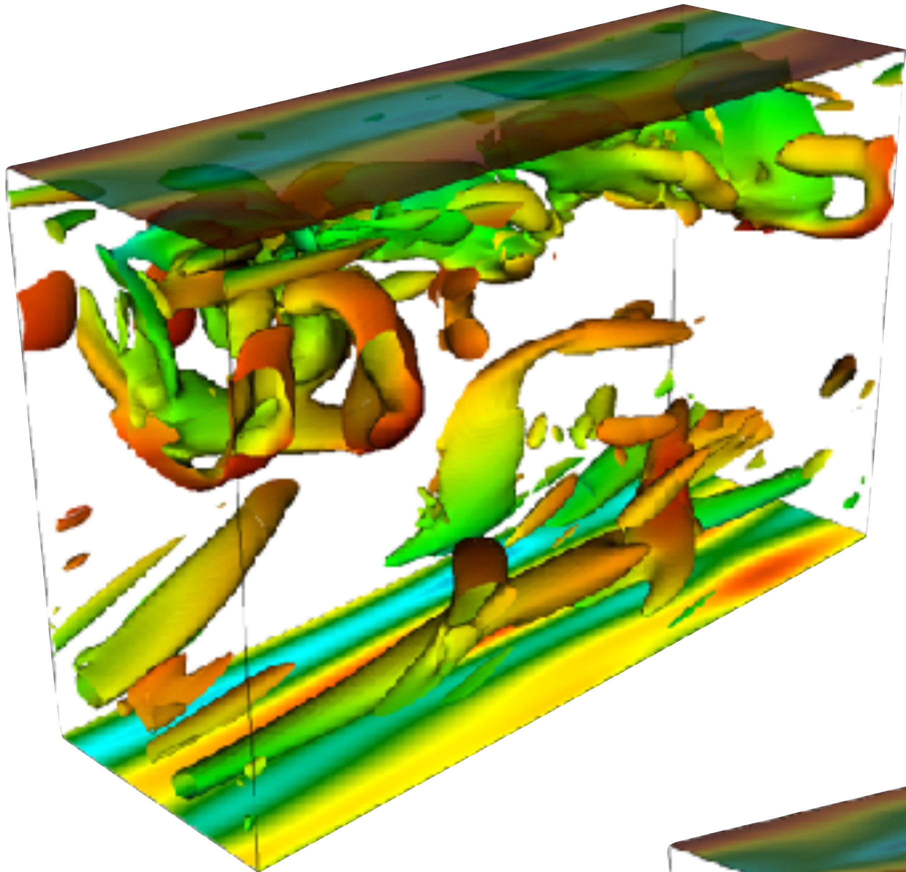
X-momentum perturbations suggested by the adjoint are similar to the optimal velocity perturbations computed by Cherubini et al.

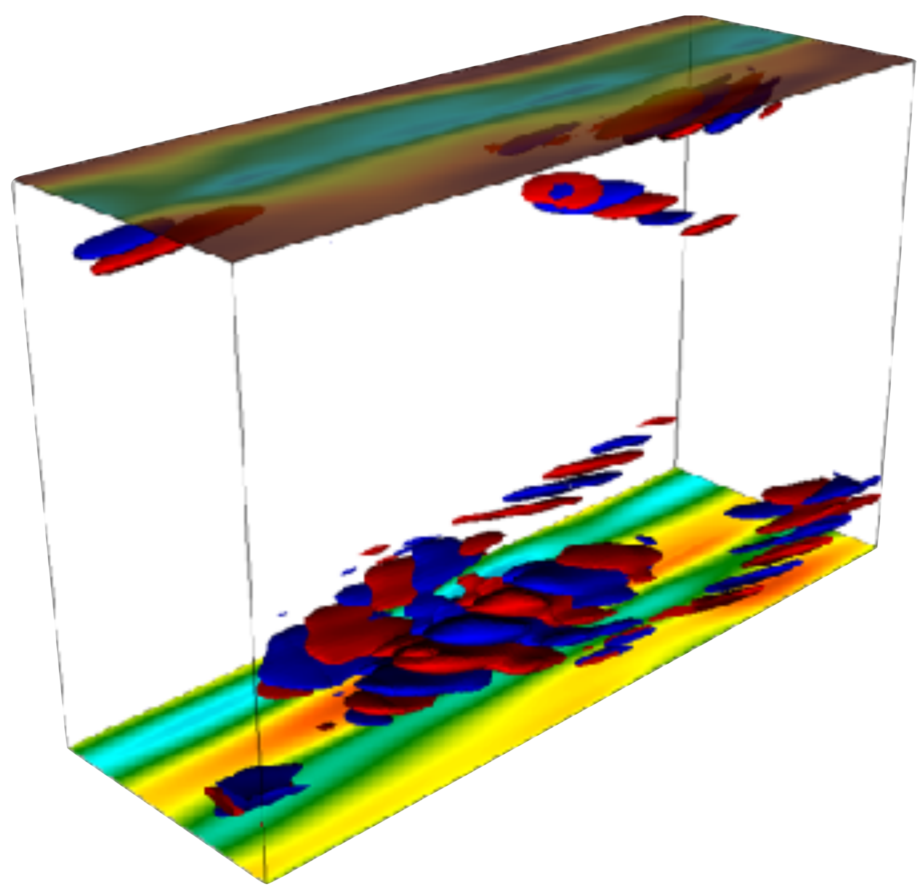
Conclusions and Future Work

- Conventional sensitivity analysis fails for chaotic dynamical systems such as scale-resolving turbulent flow simulations
- Shadowing-based sensitivity analysis is a promising approach for chaotic systems
- Non-Intrusive LSS can compute useful sensitivities
  - Cost scales with the number of positive Lyapunov exponents
- Shadowing adjoint provides valuable physical insights into turbulent flows

- Next Steps:
  - Shadowing for other canonical turbulent flows including axis-symmetric jets
  - Explore approaches to reduce cost of NILSS
  - Study other shadowing algorithms such as multiple shooting shadowing

Acknowledgments





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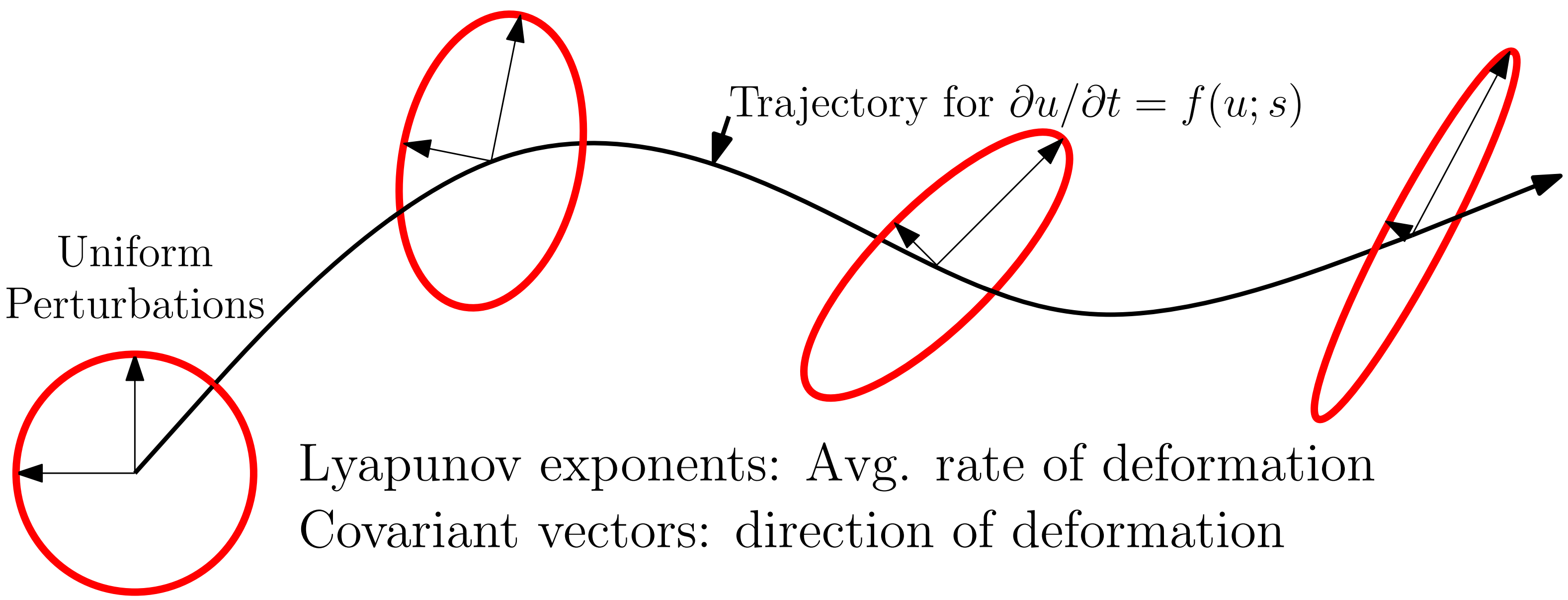
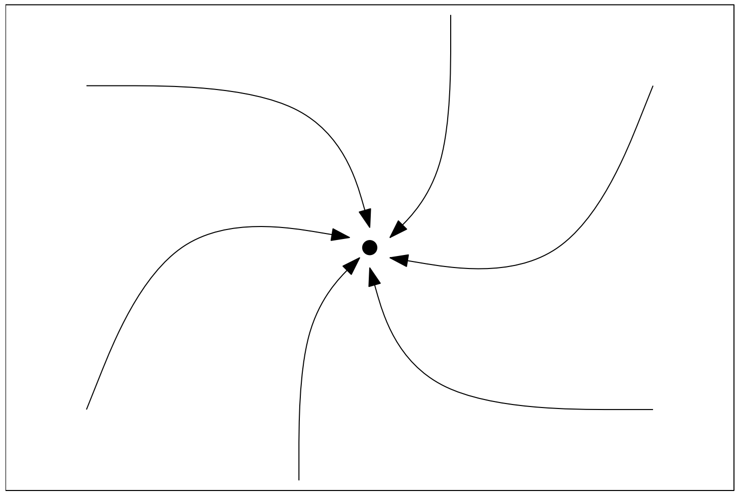
Lyapunov Analysis

- Phase Space for system $\dfrac{du}{dt} = f(u;s)$:



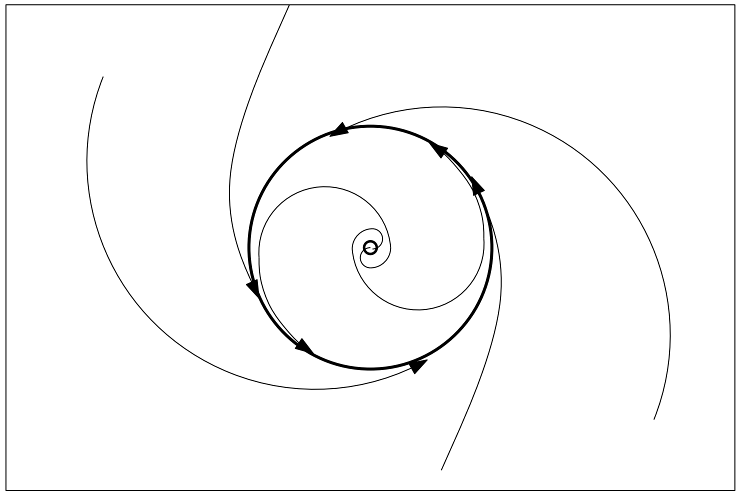
Exponent signs indicate long-time dynamics:

Steady



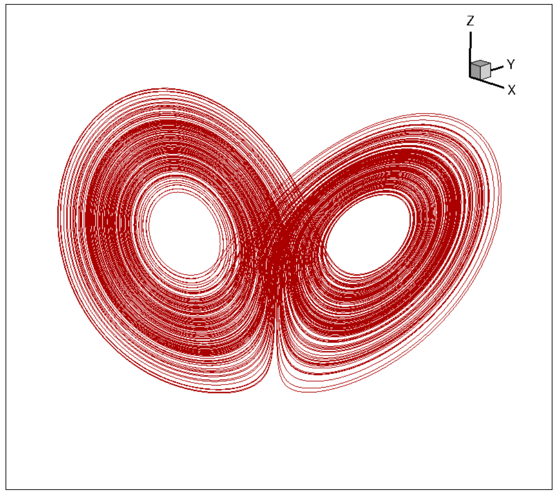
All Negative

Periodic



Zero, Negative

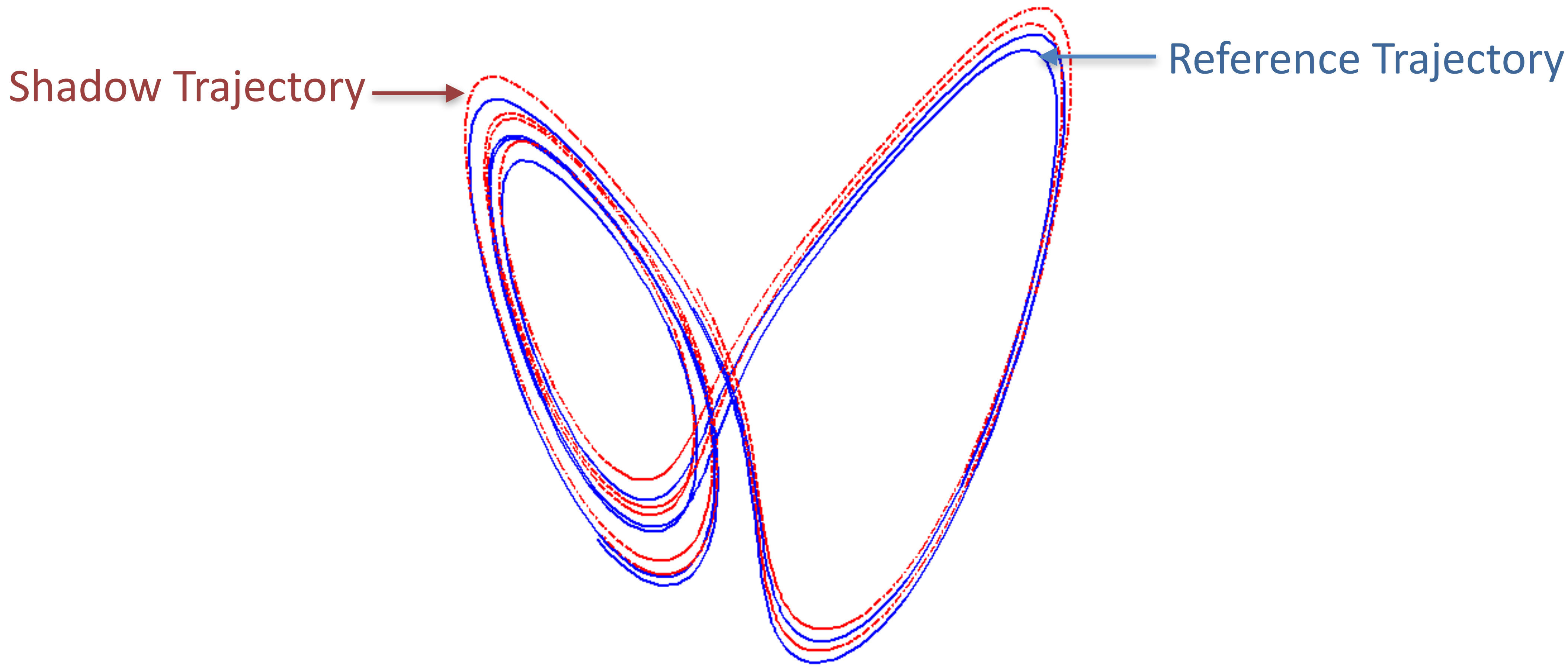
Chaotic



Positive, Zero, Negative

Positive Lyapunov exponents responsible for the butterfly effect

The Shadowing Lemma

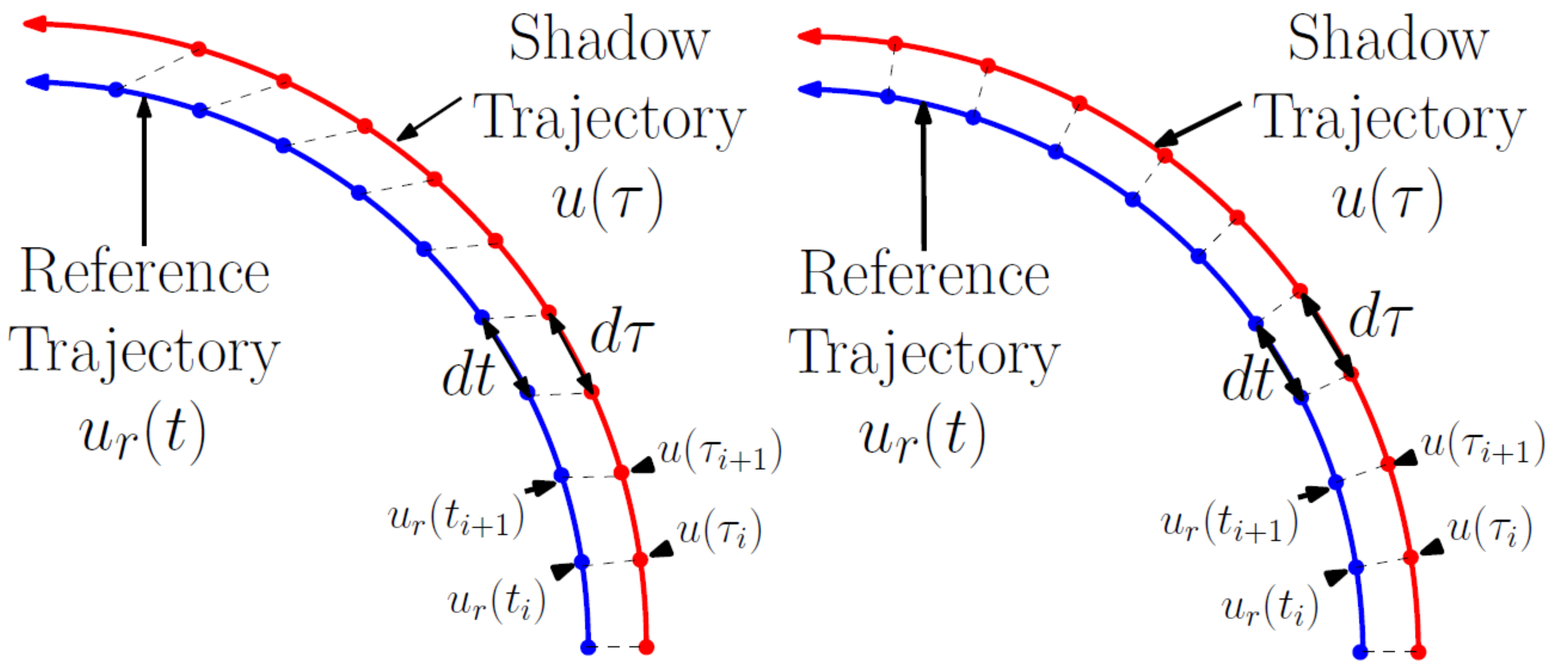


Consider a system governed by

$$\frac{du}{dt} = f(u; s)$$

For any δ>0 there exists ε>0, such that for every "ε-pseudo-solution" u satisfying ‖du/dt−f(u)‖<ε, there exists a true solution **u** satisfying d**u**/dτ−f(**u**)=0 under a time transformation τ(t), such that *‖**u**(τ)−u(t)‖<δ, |1−dτ/dt|<δ*

Time Transformation



Without Transformation

$$\frac{d\tau}{dt} = 1$$

With Transformation

$$\frac{d\tau}{dt} \neq 1$$

- Time transformation is required to keep the trajectories close in phase space for all time

Additional NILSS Definitions

- Tangent:

$$\frac{d\tilde{v}_j}{dt} = \frac{\partial f}{\partial u}\tilde{v}_j, \quad \tilde{v}_j(t_i) = V_i^j \qquad\qquad \frac{d\hat{v}}{dt} = \frac{\partial f}{\partial u}\hat{v} + \frac{\partial f}{\partial s} + \eta f, \quad \hat{v}(t_i) = \hat{V}_i$$

Sensitivity:

$$\frac{d\bar{J}}{ds} = \frac{1}{t_K - t_0}\sum_{i=1}^{K}\left({g_i}^T\alpha_i + h_i\right) + \frac{\partial \bar{J}}{\partial s}$$

- Adjoint:

$$-\frac{dw}{dt} = \left[\frac{\partial f}{\partial u}\right]^T w + \frac{1}{t_K - t_0}\frac{\partial J}{\partial u} \qquad\qquad w(t_i^-) = P_{t_i}\left((\mathcal{I} - \mathcal{Q}_i\mathcal{Q}_i^T)w(t_i^+) - \mathcal{Q}_i\psi_i\right) + x_i$$

Sensitivity:

$$\frac{d\bar{J}}{ds} = \int_{t_0}^{t_K}\left.\frac{\partial f}{\partial s}\right|_t w(t)\ dt + \frac{\partial \bar{J}}{\partial s}$$

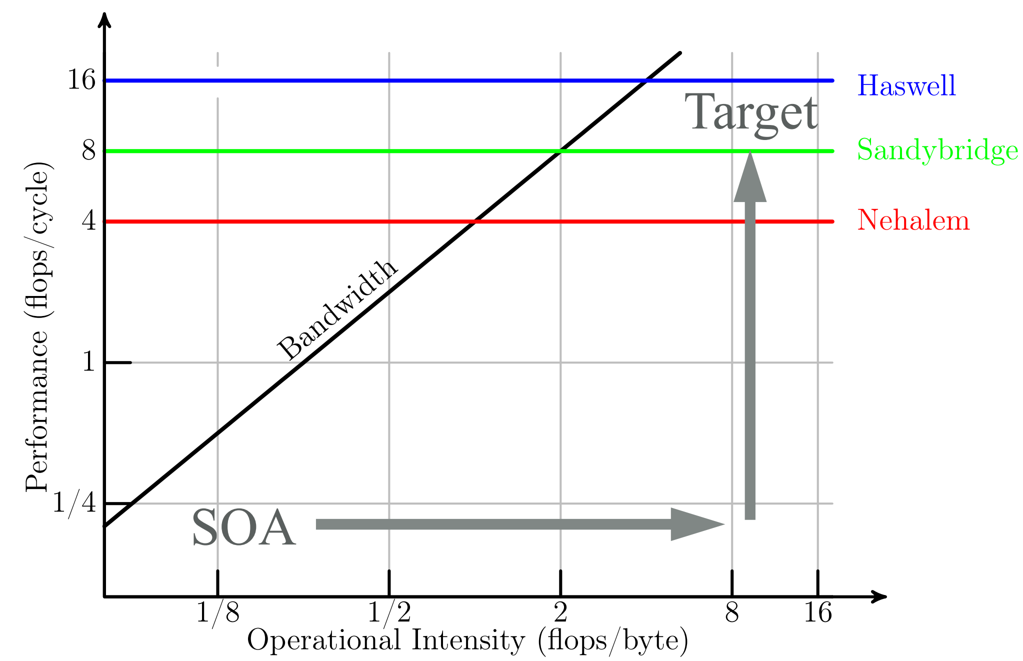
- Definitions:

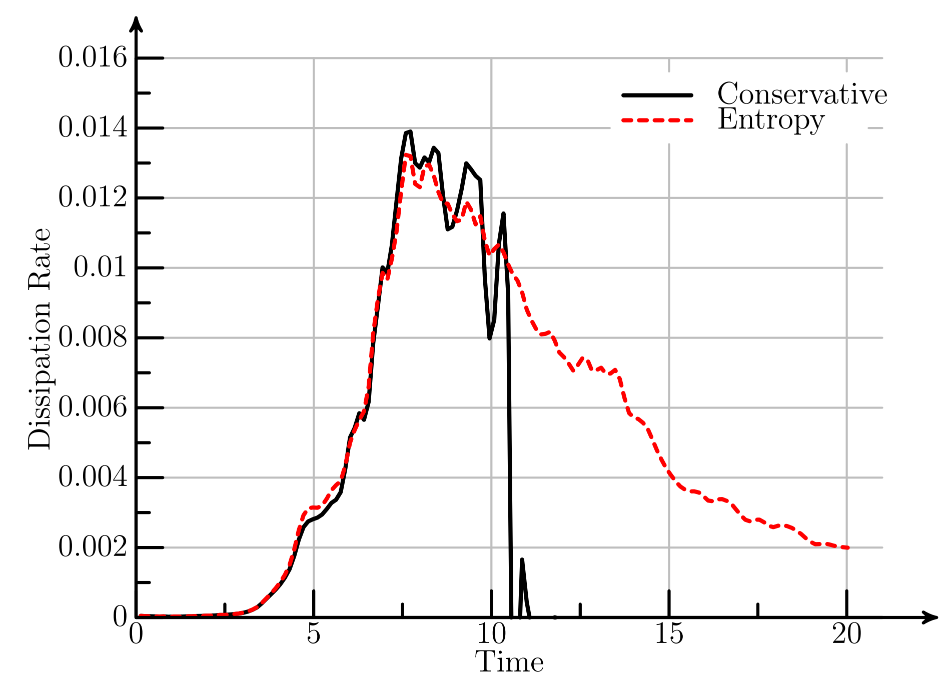
$$g_i = \frac{1}{t_K - t_0}\int_{t_{i-1}}^{t_i}\left.\frac{\partial J}{\partial u}\right|_t V(t)\ dt + x_i^T V_i^- \qquad\qquad h_i = \frac{1}{t_K - t_0}\int_{t_{i-1}}^{t_i}\left.\frac{\partial J}{\partial u}\right|_t \hat{v}(t)\ dt + x_i^T \hat{v}(t_i^-)$$

$$x_i = \frac{1}{t_K - t_0}(\bar{J} - J(u(t_i)))\frac{f(u(t_i);s)}{\|f(u(t_i);s)\|_2^2} \qquad\qquad P_{t_i} = \mathcal{I} - f(u(t_i);s)\frac{f(u(t_i);s)^T}{\|f(u(t_i);s)\|_2^2}$$

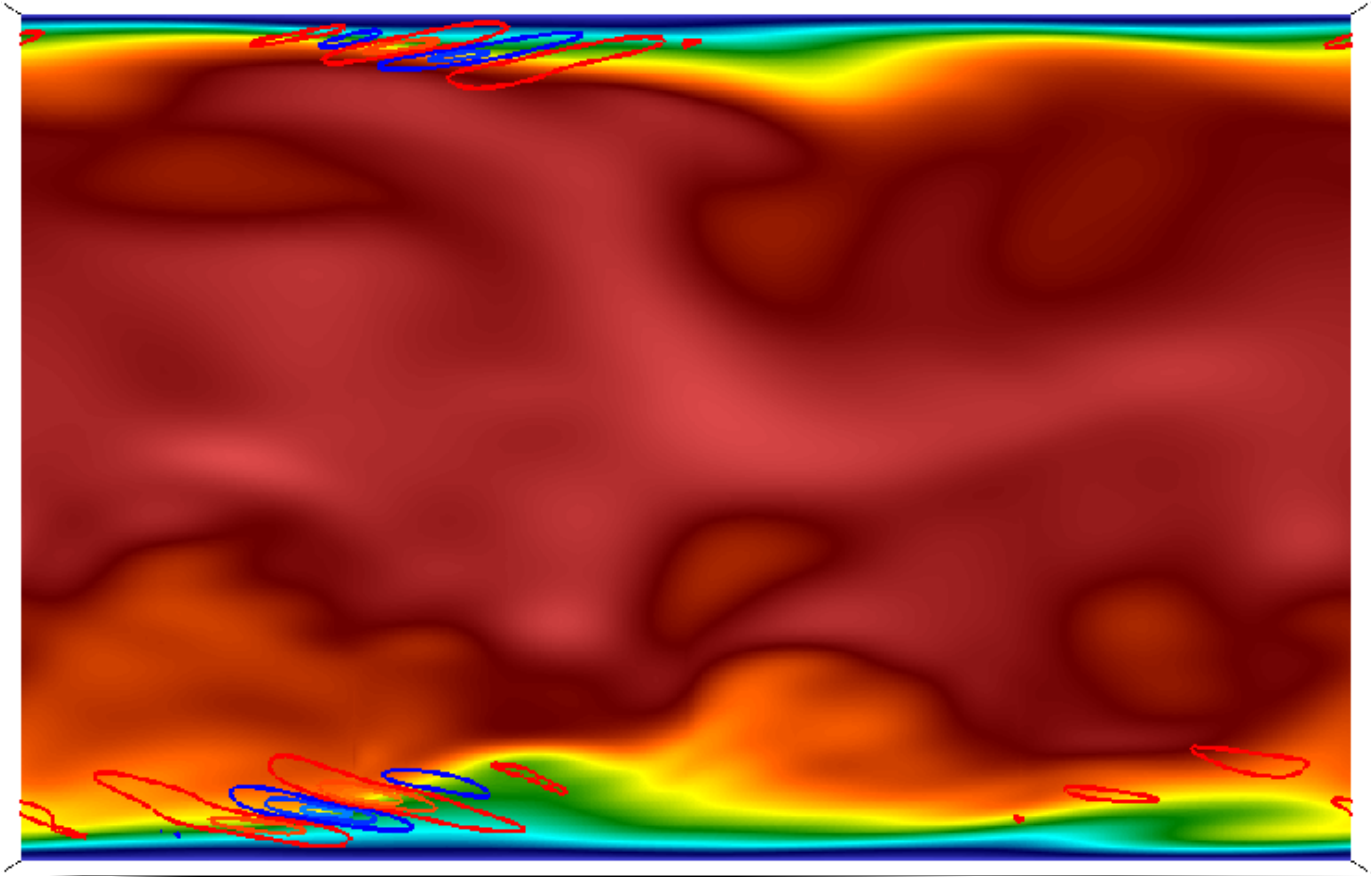
Development of a compressible **entropy-stable high-order space-time discontinuous Galerkin spectral element** method (DGSEM) framework

- DGSEM to efficiently reach spectral limit both in space and time (N ≥ 8)
  - Less discretization errors and efficiency
  - Better match for current/future hardware
  - Low dependance on mesh quality
  - *h-p* adaptation
- Entropy-stable formulation
  - Entropy variables
  - Space-time DG discretization
  - Entropy stable flux of Ismail and Roe
  - “Exact” quadrature using local de-aliasing





Flow Unit Adjoint Field



Contour lines: X-momentum adjoint
Color map: X-mometum

- Adjoint for integrated kinetic energy shows when and where flow is most susceptible to flow instabilities